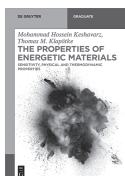


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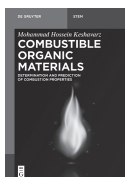
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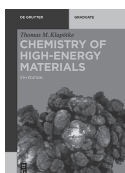
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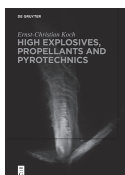


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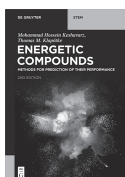


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Thomas M. Klapötke

Energetic Materials Encyclopedia

O–Z

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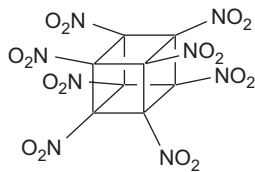
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O

Octanitrocubane

Name [German, acronym]: Octanitrocubane [octanitrocuban, ONC]
Main (potential) use: Insensitive (high) explosive, patented as potential oxidizer in PBXs^[9]
Structural formula:



	ONC
Formula	C ₈ N ₈ O ₁₆
Molecular mass [g mol ⁻¹]	464.1
Appearance at room temperature (RT)	White solid granular powder ^[9] , white solid, solvent-free crystals from trifluoroacetic acid, fuming acid/sulfuric acid or anhydrous cyclohexane ^[12]
IS [J]	Samples not detonated by hammer taps ^[12]
N [%]	24.14
Ω(CO ₂) [%]	±0
T _{m,p.} [°C]	297 (with dec.) ^[9]
T _{sublimation} [°C]	Sublimes unchange @ 200 °C @ atmospheric pressure ^[12]
T _{dec.} [°C]	297 (melts with dec.) ^[9]
ρ [g cm ⁻³]	1.979 ^[12] , 2.80 (@ 293 K) ^[1] , 2.03 (@ 294 K) ^[2] , 2.1 (theoretical), 1.92–2.2 (theoretical density) ^[9] , 2.1 (predicted using calculations for the most stable polymorph of ONC) ^[12] , 2.189 (crystal, calcd.) ^[13]
Heat of formation	413.8 kJ/mol (Δ _f H°), 81 cal/mol (Δ _f H°, calcd., est. using bond energies) ^[1, 8] , 381.2 kJ/mol (Δ _f H°) ^[3, 11] , 937 kJ/kg (Δ _f H°) ^[6] , 163 kJ/mol ^[9] , 594.1 kJ/mol (Δ _f H°) ^[10] , 374.4 kJ/mol (condensed phase enthalpy of form., calcd., EDPHT 2.0) ^[11] , 575.5 kJ/mol (condensed phase enthalpy of form., calcd., quantum mechanical) ^[11] , 594 kJ/mol (solid ONC) ^[12] , 505.84 kJ/mol (calcd.) ^[13] , 726.47 kJ/mol (calcd., gas phase) ^[13]

	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.																
$-\Delta_{\text{ex}}U^{\circ}$ [kJ kg ⁻¹]	7,376	<div>7,271 (calcd.)^[6]</div> <div>ONC $\rho = 2.09$ g/cm³, $\Delta H_{\text{f}}^{\circ} = 594.1$ kJ/mol (* = @ $Q_{\text{calc}} = Q_{\text{max}}$)^[10]:</div> <table><tr><td>Calcd. method</td><td>Q_{calc}, MJ/kg</td></tr><tr><td>Lit. method</td><td>8.07</td></tr><tr><td>BKW-RDX</td><td>7.99</td></tr><tr><td>BKW-R</td><td>7.94</td></tr><tr><td>BKW-RR</td><td>7.87</td></tr><tr><td>Lit. method</td><td>8.06</td></tr><tr><td>Lit. method</td><td>7.63</td></tr><tr><td>Lit. method</td><td>8.06*</td></tr></table>	Calcd. method	Q_{calc} , MJ/kg	Lit. method	8.07	BKW-RDX	7.99	BKW-R	7.94	BKW-RR	7.87	Lit. method	8.06	Lit. method	7.63	Lit. method	8.06*	
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BKW-RR	7.87																		
Lit. method	8.06																		
Lit. method	7.63																		
Lit. method	8.06*																		
T_{ex} [K]	5,324	<div>ONC $\rho = 2.09$ g/cm³, $\Delta H_{\text{f}}^{\circ} = 594.1$ kJ/mol^[10]:</div> <table><tr><td>Calcd. method</td><td>T_{CJ}, K</td></tr><tr><td>BKW-RDX</td><td>3,325</td></tr><tr><td>BKW-R</td><td>4,849</td></tr><tr><td>BKW-RR</td><td>4,798</td></tr></table>	Calcd. method	T_{CJ} , K	BKW-RDX	3,325	BKW-R	4,849	BKW-RR	4,798									
Calcd. method	T_{CJ} , K																		
BKW-RDX	3,325																		
BKW-R	4,849																		
BKW-RR	4,798																		
$p_{\text{C-J}}$ [kbar]	422	<div>390 (calcd.)^[6]</div> <div>467 (@ 2.10 g cm⁻³, calcd., K-J simple method)^[1]</div> <div>467 (@ 2.09 g cm⁻³, calcd., K-J simple method)^[8]</div> <div>520.85 (@ 2.189 g cm⁻³, calcd., $\Delta H_{\text{f}}^{\circ} = 505.84$ kJ/mol)^[13]</div> <div>ONC $\rho = 2.09$ g/cm³, $\Delta H_{\text{f}}^{\circ} = 594.1$ kJ/mol († = @ single crystal density d_{4}^{20} of 2.11 g/cm³, * = @ $Q_{\text{calc}} = Q_{\text{max}}$)^[10]:</div>																	

		<table><tr><td>Calcd. method</td><td>ρ_{CJ}, GPa</td></tr><tr><td>Lit. method</td><td>46.9</td></tr><tr><td>BKW-RDX</td><td>49.8</td></tr><tr><td>BKW-R</td><td>46.6</td></tr><tr><td>BKW-RR</td><td>44.8</td></tr><tr><td>Lit. method</td><td>37.7[†]</td></tr><tr><td>Lit. method</td><td>48.0</td></tr><tr><td>Lit. method</td><td>50.7</td></tr><tr><td>Lit. method</td><td>41.2*</td></tr></table>	Calcd. method	ρ_{CJ} , GPa	Lit. method	46.9	BKW-RDX	49.8	BKW-R	46.6	BKW-RR	44.8	Lit. method	37.7 [†]	Lit. method	48.0	Lit. method	50.7	Lit. method	41.2*	
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Lit. method	50.7																				
Lit. method	41.2*																				
VoD [m s ⁻¹]	9,562 (@ TMD)	<p>9,350 (@ 1.982 g cm⁻³, calcd.)^[6]</p> <p>9,900 (calcd.)^[2]</p> <p>9,820 (@ 2.09 g cm⁻³, calcd., K-J simple method)^[8]</p> <p>1,026 (@ 2.189 g cm⁻³, calcd., $\Delta H_f = 505.84$ kJ/mol)^[13]</p> <p>ONC $\rho = 2.09$ g/cm³, $\Delta H_f^\circ = 594.1$ kJ/mol ([†] = @ single crystal ρ d^{20}_4 of 2.11 g/cm³, * = @ $Q_{\text{calc}} = Q_{\text{max}}$)^[10]:</p> <table><tr><td>Calcd. method</td><td>D, km/s</td></tr><tr><td>Lit. method</td><td>9.20</td></tr><tr><td>BKW-RDX</td><td>9.90</td></tr><tr><td>BKW-R</td><td>9.51</td></tr><tr><td>BKW-RR</td><td>9.31</td></tr><tr><td>Lit. method</td><td>8.93[†]</td></tr><tr><td>Lit. method</td><td>9.97</td></tr><tr><td>Lit. method</td><td>10.16</td></tr><tr><td>Lit. method</td><td>8.95*</td></tr></table>	Calcd. method	D , km/s	Lit. method	9.20	BKW-RDX	9.90	BKW-R	9.51	BKW-RR	9.31	Lit. method	8.93 [†]	Lit. method	9.97	Lit. method	10.16	Lit. method	8.95*	<p>9,800 (@ 2.00 g cm⁻³)^[5]</p> <p>10,100 (@ 2.00 g cm⁻³)^[7]</p>
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Lit. method	9.20																				
BKW-RDX	9.90																				
BKW-R	9.51																				
BKW-RR	9.31																				
Lit. method	8.93 [†]																				
Lit. method	9.97																				
Lit. method	10.16																				
Lit. method	8.95*																				
V_0 [L kg ⁻¹]	646																				

I_{rel}		ONC $\rho = 2.09 \text{ g/cm}^3$, $\Delta H_f^\circ = 594.1 \text{ kJ/mol}$ ($^\dagger = @$ single crystal $\rho_{d^{20}_4}$ of 2.11 g/cm^3 , $^* = @ Q_{\text{calc}} = Q_{\text{max}})^{[10]}$;																			
		<table><tr><th>Calcd. method</th><th>I_{rel}</th></tr><tr><td>Lit. method</td><td>146.7</td></tr><tr><td>BKW-RDX</td><td>144.9</td></tr><tr><td>BKW-R</td><td>140.9</td></tr><tr><td>BKW-RR</td><td>138.3</td></tr><tr><td>Lit. method</td><td>121.6†</td></tr><tr><td>Lit. method</td><td>138.7</td></tr><tr><td>Lit. method</td><td>146.6</td></tr><tr><td>Lit. method</td><td>124.4*</td></tr></table>	Calcd. method	I_{rel}	Lit. method	146.7	BKW-RDX	144.9	BKW-R	140.9	BKW-RR	138.3	Lit. method	121.6 †	Lit. method	138.7	Lit. method	146.6	Lit. method	124.4 *	
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Lit. method	138.7																				
Lit. method	146.6																				
Lit. method	124.4 *																				

Thermal stability	Little known about long-term storage behavior ^[12] , at least one sample sealed in glass tube survived unchanged for 14 months ^[12]																		
Enthalpy of sublimation [kJ/mol]	220.63 (calcd.) ^[13]																		
Activation energy for pyrolysis initiation reaction [kJ/mol]	155.30 (calcd.) ^[13]																		
Heat capacity [J•mol ⁻¹ •K ⁻¹]	Calcd. standard molar heat capacity, T in K, data from ^[13] : <table><tr><th>T (K)</th><th>$C_{p,m}^\circ$</th></tr><tr><td>298</td><td>411.86</td></tr><tr><td>400</td><td>492.60</td></tr><tr><td>500</td><td>554.97</td></tr><tr><td>600</td><td>602.25</td></tr><tr><td>700</td><td>637.73</td></tr><tr><td>800</td><td>664.47</td></tr><tr><td>900</td><td>684.85</td></tr><tr><td>1,000</td><td>700.60</td></tr></table>	T (K)	$C_{p,m}^\circ$	298	411.86	400	492.60	500	554.97	600	602.25	700	637.73	800	664.47	900	684.85	1,000	700.60
T (K)	$C_{p,m}^\circ$																		
298	411.86																		
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600	602.25																		
700	637.73																		
800	664.47																		
900	684.85																		
1,000	700.60																		

	ONC^[4]
Chemical formula	C ₈ N ₈ O ₁₆
Molecular weight [g mol ⁻¹]	130.06
Crystal system	Monoclinic
Space group	C2/c (No. 15)
<i>a</i> [Å]	12.785(1)
<i>b</i> [Å]	8.840(1)
<i>c</i> [Å]	13.924(1)
α [°]	90
β [°]	98.03
γ [°]	90
<i>V</i> [Å ³]	1,558.17
<i>Z</i>	4
ρ_{calc} [g cm ⁻³]	1.978
<i>T</i> [K]	283–303

Solvent-free crystals from trifluoroacetic acid, fuming acid/sulfuric acid or anhydrous cyclohexane.^[12]

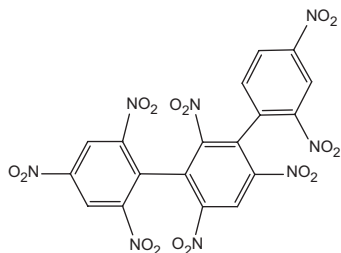
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Octanitroterphenyl

Name [German, acronym]: 2,2^I,4,4^I,4^{II},6,6^I,6^{II}-Octanitro-*m*-terphenyl,
2,2'',4,4',4'',6,6',6''-octanitro-1,1':3',1''-terphenyl
[oktanit, ONT]

Main (potential) use: Thermally highly stable secondary explosive,
components of perforators or detonators in downhole
well applications, possible spacecraft applications

Structural formula:



	ONT															
Formula	C ₁₈ H ₆ N ₈ O ₁₆															
Molecular mass [g mol ⁻¹]	590.31															
Appearance at RT																
IS [J]	$H_{50} = 3.85^{[1]}$, 15.73 (Bruceton) ^[8] , $H_{50} = 40$ cm (2.5 kg mass, type 12 tool) ^[11] , $H_{50\%} = 64$ cm (type 12 tool, 2.5 kg mass, sandpaper) ^[16]															
FS [N]	$F_{50} > 36$ kgf ^[1]															
ESD [J]	$E_{50} = 0.887$ (@ 293 K) ^[1] , $E_{50} = 0.940$ (@ 333 K) ^[1] , $E_{50\%} = 0.887$ ($T_0 = 293$ K) ^[1] , 0.940 ($T_0 = 333$ K) ^[1] Data from ^[16] : ESD (NAVORD OD 44811), test conditions = 10 K Volt potential, 0.01 mfd capacitance, result = ONT passed* (*observation of 20 consecutive shots with no smoke, burning and/or explosion) ^[16] Data from ^[16] (*observation of 20 consecutive shots with no smoke, burning and/or explosion): <table><tr><td>Capacitance (mfd)</td><td>m/m</td><td>m/r</td></tr><tr><td>1.0</td><td>–</td><td>–</td></tr><tr><td>0.1</td><td>–</td><td>3,000</td></tr><tr><td>0.01</td><td>7,400</td><td>7,500*</td></tr><tr><td>0.001</td><td>7,500</td><td>7,500*</td></tr></table>	Capacitance (mfd)	m/m	m/r	1.0	–	–	0.1	–	3,000	0.01	7,400	7,500*	0.001	7,500	7,500*
Capacitance (mfd)	m/m	m/r														
1.0	–	–														
0.1	–	3,000														
0.01	7,400	7,500*														
0.001	7,500	7,500*														

N [%]	18.98		
$\Omega(\text{CO}_2)$ [%]	−62.34		
$T_{\text{m.p.}}$ [°C]	>400 ^[5, 10] , 362 (dec.) ^[7] , 387.5 (dec., sample in sealed cell) ^[1]		
$T_{\text{dec.}}$ [°C]	387.5 (DSC, sample in sealed cell) ^[1] , 334 (DTA, onset exotherm) ^[8, 12]		
ρ [g cm ^{−3}]	1.80 (@ TMD) ^[1] , 1.80 ^[3]		
Heat of formation	19.7 kcal mol ^{−1} ^[3] , 99.2 kcal/kg (ΔH_f) ^[1] , 38.0 kcal/kg (enthalpy of form.) ^[9] , 19.7 kcal/mol (ΔH°_f) ^[15] , 94.6 kJ/mol (enthalpy of form., exptl.) ^[14] , 105.4 kJ/mol (enthalpy of form., calcd., emp.) ^[14] , 94.7 kJ/mol (enthalpy of form., calcd., S-D method) ^[14]		
Heat of combustion	−1,917.6 kcal mol ^{−1} ^[3] , $\Delta H^\circ_c = -1,917.6$ kcal/mol ^[15]		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^\circ$ [kJ kg ^{−1}]		4,550 MJ•kg ^{−1} (@ TMD, Q_{real}) ^[12] 1,035 kcal/kg (@ 1.490 g cm ^{−3} , calcd.) [H ₂ O vapor] ^[9]	1,039 kcal/kg (@ 1.490 g cm ^{−3}) [H ₂ O vapor] ^[9]
T_{ex} [K]			
$p_{\text{C-J}}$ [kbar]		247 (calcd. K-J) ^[3]	
VoD [m s ^{−1}]		7,460 (@ 1.80 g cm ^{−3} , calcd. K-J) ^[3, 8] 7,310 (@ 1.78 g cm ^{−3} , calcd. empirical, Rothstein method) ^[4] 7,460 (@ TMD, calcd., K-J) ^[12]	7,330 (no ρ given) ^[3, 4] 7,330 (@ 1.800 g cm ^{−3}) ^[6] 7,200 (@ 1.72 g cm ^{−3}) ^[8, 12]
V_0 [L kg ^{−1}]			

SSGT [cm]	L_c (critical length) = 8 mm (critical length, underwater SSGT) ^[1] Data from ^[16] : <table><tr><th rowspan="2">Loading pressure (kpsi)</th><th colspan="2">Density (g/cm³)</th><th colspan="4">Sensitivity (DBG)</th></tr><tr><th>Avg.</th><th><i>s</i></th><th>Avg.</th><th><i>g</i></th><th><i>S_m</i></th><th><i>N</i></th></tr><tr><td>4</td><td>1.396</td><td>0.0113</td><td>4.567</td><td>0.0617</td><td>0.03489</td><td>20</td></tr><tr><td>8</td><td>1.487</td><td>0.0082</td><td>4.752</td><td>0.0068</td><td>0.0070</td><td>20</td></tr><tr><td>16</td><td>1.595</td><td>0.0068</td><td>5.213</td><td>0.0071</td><td>0.0039</td><td>20</td></tr><tr><td>32</td><td>1.6775</td><td>0.0045</td><td>5.950</td><td>–</td><td>–</td><td>20</td></tr><tr><td>64</td><td>1.7688</td><td>0.0038</td><td>6.936</td><td>0.0276</td><td>0.0219</td><td>20</td></tr></table>	Loading pressure (kpsi)	Density (g/cm ³)		Sensitivity (DBG)				Avg.	<i>s</i>	Avg.	<i>g</i>	<i>S_m</i>	<i>N</i>	4	1.396	0.0113	4.567	0.0617	0.03489	20	8	1.487	0.0082	4.752	0.0068	0.0070	20	16	1.595	0.0068	5.213	0.0071	0.0039	20	32	1.6775	0.0045	5.950	–	–	20	64	1.7688	0.0038	6.936	0.0276	0.0219	20
Loading pressure (kpsi)	Density (g/cm ³)		Sensitivity (DBG)																																														
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32	1.6775	0.0045	5.950	–	–	20																																											
64	1.7688	0.0038	6.936	0.0276	0.0219	20																																											
5 s explosion <i>T</i> [°C] Ignition <i>T</i> [°C]	370 ^[8, 12]																																																
Thermal stability	290 °C (threshold of thermal stability) ^[8, 12] Analysis of explosives after heat treatment under vacuum ^[16] : <table><tr><th>Explosive</th><th><i>T</i> (°C)</th><th>Time (h)</th><th>% Explosive in residue</th></tr><tr><td>ONT</td><td>278</td><td>16</td><td>96.7</td></tr><tr><td>ONT</td><td>250</td><td>44</td><td>98.7</td></tr></table>	Explosive	<i>T</i> (°C)	Time (h)	% Explosive in residue	ONT	278	16	96.7	ONT	250	44	98.7																																				
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ONT	278	16	96.7																																														
ONT	250	44	98.7																																														
Vacuum stability test [cm ³ /days]	@ 200 °C (total amount of gas evolved): 0.9/2, 1.3/7, 1.4/14, 1.5/21, 1.6/28, 1.7/35, 1.9/42, 1.9/49, 2.0/56, 2.1/63, 2.3/70, 2.4/77, 2.5/84, 2.6/91 ^[2, 13] @ 175 °C (total amount of gas evolved): 0.2/2, 0.6/7, 0.9/14, 1.2/21, 1.3/28, 1.4/35, 1.5/42, 1.6/49, 1.7/56, 1.8/63, 1.9/70, 1.9/77, 2.0/84, 2.0/91 ^[2] @ 150 °C (total amount of gas evolved): 0.1/2, 0.2/7, 0.2/14, 0.3/21, 0.4/28, 0.4/35, 0.5/42, 0.6/49, 0.6/56, 0.7/63, 0.8/70, 0.8/77, 0.9/84, 0.9/91 ^[2] Data from ^[16] : <table><tr><th>Explosive</th><th><i>T</i> (°C)</th><th>20 min surge (cc/g)</th><th>2 h period (cc/g/h)</th></tr><tr><td>ONT</td><td>280</td><td>0.28</td><td>0.63</td></tr><tr><td>ONT (NOL ID 1803)</td><td>300</td><td>0.88</td><td>3.94</td></tr></table>	Explosive	<i>T</i> (°C)	20 min surge (cc/g)	2 h period (cc/g/h)	ONT	280	0.28	0.63	ONT (NOL ID 1803)	300	0.88	3.94																																				
Explosive	<i>T</i> (°C)	20 min surge (cc/g)	2 h period (cc/g/h)																																														
ONT	280	0.28	0.63																																														
ONT (NOL ID 1803)	300	0.88	3.94																																														

Vapor pressure [atm. @ °C]	Summary of data obtained and vapor pressures calculated in the vapor pressure study ^[16] :				
	<i>T</i> (°C)	Δt (s)	Surface area (cm ²)	Wt. loss (g)	Vapor pressure (torr)
	277.8	38,400	5.1	0.1760	1.50(10 ⁻⁵)
	247.6	56,220	6.3	0.0189	8.57(10 ⁻⁷)
	247.6	55,200	5.1	0.0185	1.07(10 ⁻⁶)
	247.6	190,920	5.1	0.0341	5.67(10 ⁻⁷)
	206.9	71,040	5.1	0.0021	9.01(10 ⁻⁸)
	206.9	229,020	5.1	0.0041	5.46(10 ⁻⁸)
	149.7	492,900	5.1	Indeterminate	
Compatibility	Data in ^[16] :				
	Sample		Compatible	@280 °C	
				20 min gas surge (cc/g)	2 h (mL/g/h)
	ONT/Ag	50/50	Yes	0.22	0.38
	ONT/Al	50/50	Yes	0.25	0.35
	ONT/Pb + Sb	50/50	Yes	0.26	0.35
	ONT/stainless steel	50/50	Yes	0.32	0.36

	ONT^[7]
Chemical formula	C ₁₆ H ₆ N ₈ O ₁₆
Molecular weight [g mol ⁻¹]	590.31
Crystal system	Orthorhombic
Space group	<i>P</i> 2 ₁ 2 ₁ 2 ₁
<i>a</i> [Å]	11.4131(9)
<i>b</i> [Å]	11.4128(5)
<i>c</i> [Å]	16.4168(12)
α [°]	90
β [°]	90
γ [°]	90
<i>V</i> [Å ³]	2,138.4

Z	4
$\rho_{\text{calc}} [\text{g cm}^{-3}]$	1.834
$T [\text{K}]$	150

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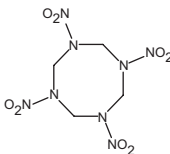
Octogen

Name [German, acronym]: β -Octogen, tetramethylenetetranitramine, 1,3,5,7-tetraza-1,3,5,7-tetranitrocyclooctane, cyclotetramethylenetetranitramine, octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine, 1,3,5,7-tetranitro-1,3,5,7-tetrazacyclooctane, homocyclonite [β -HMX]*

*(Values given are for β -HMX unless otherwise stated: Note - although values have been included for γ -HMX, it is has been determined that γ -HMX is in fact a hydrate and not a true polymorph of HMX).

Main (potential) use: Secondary (high) explosive, high performance solid propellant, ingredient in plastic-bonded explosives[†], explosive charge when desensitized^[16], booster charge with TNT in Octols^[16], oxidizer in solid rocket and gun propellants^[16]

Structural formula:



[†] Military-grade HMX consists of only the β -polymorph^[16]

	β -HMX
Formula	$C_4H_8N_8O_8$
Molecular mass [g mol ⁻¹]	296.16
Appearance at RT	β -HMX: white transparent crystals on recryst. from acetone/acetonitrile ^[130] , γ -HMX: fluffy white powder/crystals ^[130] , white crystalline material ^[137] , white crystals ^[139] , white solid ^[14, 147] , white, crystalline solid ^[16] , solid light crystalline substance, large, transparent, rhombic crystals if slowly recryst. from acetone ^[150]
IS [J]	6.40 ^[1] , 7.4 Nm ^[3] , 7.59 (1st reaction) ^[6, 82] , 6.40 (sound) ^[6, 82] , 6.35 (20 μ m) ^[8] , 6.55 (50 μ m) ^[8] , 6.65 (100 μ m) ^[8] , 6.88 (200 μ m) ^[8] , 9.17 (300 μ m) ^[8] , 10.72 (400 μ m) ^[8] , 6.37 ^[9] , 60 cm (B.M.) ^[12, 13] , 23 cm (P.A.) ^[12, 13] , 26 cm (tool type 12, E.R.L.) ^[12, 13] , 33 cm (tool type 12, 5 kg mass, E.R.L.) ^[12, 13] , 32 cm (32 mg sample, B.M.) ^[14] , 9 in (23 mg sample, P.A.) ^[14] , 32 cm (2 kg mass, B.M.) ^[16] , H_{50} = 26 cm (tool type 12) ^[17] , H_{50} = 37 cm (tool type 12B) ^[17] , H_{50} = 33 cm

(tool type 12, 5 kg mass)^[21], $H_{50} = 40$ cm (tool type 12B, 5 kg mass)^[21], $H_{50\%} = 26$ cm (US-NOL apparatus)^[28, 29], $H_{50\%} = 26$ cm (LASL test)^[23], 32 cm (20 mg sample, 2 kg mass, B.M.)^[27], 9 in (23 mg sample, 2 kg mass, P.A.)^[27], median height = 73 cm (5 kg mass, 30 mg sample, Rotter apparatus)^[29], $H_{50\%} = 26$ cm (LASL)^[29], $H_{10\%} = 32$ cm (B.M.)^[29], $H_{10\%} = 9$ in (P.A.)^[29], 4.0 Nm (BAM)^[34], 7.59 (drop energy required for 50% initiation probability, 25 mg sample, Julius-Peters apparatus)^[33], Rotter FOI = 49–55 (powdered sample)^[38], 30–35 cm (US drop-hammer)^[38], 6.2 (micro-HMX)^[164], 6.6 (submicro-HMX)^[164], $A_{d1} = 92\%$, $A_{d2} = 100\%$, $LL = 0.7$ m, $A_{50\ d1} = 1.8$ m, $A_{50\ d2} = 0.8$ ^[19], 31–32 cm (β -HMX, Holston Defense Corp., 5 kg mass)^[174], 5–50 cm (α -HMX, Holston Defense Corp., 5 kg mass)^[174], 6–25 cm (δ -HMX, Holston Defense Corp., 5 kg mass)^[174], 6–12 cm (γ -HMX, Holston Defense Corp., 5 kg mass)^[174]

Sensitivity: $\delta > \gamma > \alpha > \beta$.^[27, 41, 174], crystal habit has a significant effect on the IS of α -HMX and γ -HMX but little effect on δ -HMX^[174]

P.A. apparatus (type 12 tool, 2.5 kg mass): δ - = 19.2 cm, γ - = 13.8–33.9 cm, α - = 15.6–22.4 cm, β - = 21.2–24.9 cm^[27]

Olin impact test apparatus^[24]:

Olin impact test apparatus			
Dropping mass (kg)	Drop height (cm)	No. of trials	No. of initiations
5.0	9	20	0
4.0	14	10	1
3.0	21	32	1
5.0	14	13	1
4.0	21	10	2
3.0	32	30	3
5.0	21	15	2
2.0	56	10	1
4.0	32	30	8
3.0	48	35	5
5.0	32	20	12
3.0	56	30	17
4.0	48	10	9
4.0	56	10	7
5.0	48	10	10

Powdered samples: $H_{50\%} = 26$ cm (NOL)^[29], $H_{50\%} = 26$ cm (LASL)^[29], $H_{10\%} = 32$ cm (B.M.)^[29], $H_{10\%} = 9$ in (P.A.)^[29], 42 (BAM, Julius-Peters)^[50], 17–25 cm (ERL)^[51], 1–8 cm (ABL)^[51], 27 in (Tc)^[51], $H_{50} = 30$ cm (2 kg hammer)^[53], $H_{50} = 16.8 \pm 0.1$ cm (FC-HMX)^[55], $H_{50} = 72.2 \pm 0.1$ cm (FD-HMX)^[55], $H_{50} = 59.6 \pm 0.1$ cm (LC-HMX)^[55], $H_{50} = 68.8 \pm 0.1$ cm (LD-HMX)^[55], 42 (BAM Julius-Peters)^[50], 17–25 cm (ERL)^[51], 1–8 cm (ABL)^[51], $H_{50} = 30$ cm (2 g hammer)^[53, 101], <7 (α -HMX (authentic), Rotter Fol, 5 kg mass, VMD 80 μ m, Rotter impact test)^[59], 60 (β -HMX (authentic), 17–23 (α -HMX (from reaction of TAT with N_2O_5/HNO_3 ; quenched with H_2O), Rotter Fol, 5 kg mass, VMD 14 μ m, Rotter impact test)^[59], 13 (α -HMX (from reaction of TAT with N_2O_5/HNO_3 ; not quenched with H_2O), Rotter Fol, 5 kg mass, VMD 12 μ m, Rotter impact test)^[59], 33–40 (α -HMX (from reaction of TAT with N_2O_5/HNO_3 ; quenched with H_2O , followed by addition of HMX/ HNO_3), Rotter Fol, 5 kg mass, VMD 24 μ m, Rotter impact test)^[59], 20–27 (α -HMX (from reaction of DADN with $N_2O_5/Ac_2O/HNO_3$ followed by quenching with H_2O), Rotter Fol, 5 kg mass, VMD 17 μ m, Rotter impact test)^[59], Rotter Fol, 5 kg mass, VMD 80 μ m, Rotter impact test)^[59], 20 cm (BAM, 2 kg mass, HMX Klasse-C)^[60], $H_{50} = 29$ cm^[63], 5.0 (β -, nonheated sample, BAM)^[65], 2.0 (δ -, sample heated @ 6 °C/min, maintained @ 200 °C for 30 min then cooled to RT, BAM)^[65], 19 cm (NEDED)^[66], 28 cm (NOL)^[22], 32 cm (LANL)^[22], 27 in (20 μ . Thiokol app.)^[67], 1.8 cm (20 μ , ABL app.)^[67], $H_{50\%} = 26$ cm (US NOL, 2.5 kg hammer, 35 mg sample)^[74], explosive layer was only partly consumed for impacts from a drop-height of 1 m (β -HMX, glass-anvil drop-weight machine, max. drop height 1.3 m, powdered sample)^[75], 3 Nm ($H_{50}Wg^{-1}$)^[77], 1.8 cm (ABL)^[80], 17–25 cm (ERL)^[80], 26 cm (Bruceton method, type 12 tool, 2.5 kg mass, 40 mg sample, 5/0 sandpaper, 25 trials)^[84], 7.5 Nm^[88], 6.0 Nm (20 °C, 42% rel. humidity, time of sample bead milling = 0 h)^[99], 6.0 Nm (20 °C, 42% rel. humidity, time of sample bead milling = 1.0 h)^[99], 6.0 Nm (20 °C, 42% rel. humidity, time of sample bead milling = 5.9 h)^[99], 7.5 Nm ($d_{50.3} = 0.58$ μ m, ball milled)^[103], 7.5 Nm ($d_{50.3} = 355$ μ m)^[103], 6.0 Nm ($d_{50.3} = 7.6$ μ m, particles processed by PCA)^[103], $H_{50} = 24.5$ cm (5 kg mass, 30 mg sample, GJB-772A-97 standard method 601.2)^[114], 10 Nm (HMX core material, mean particle size = 197 μ m)^[117], 7.5 Nm (pure HMX after 3 h fluidized bed process, mean particle size = 75 μ m (abrasion))^[117], 17 cm (minimum, 2.5 kg mass, type 12 tool, HMX grade B, composition: β -HMX = $\geq 98\%$ by weight, α -HMX = $\leq 0.01\%$ by weight, RDX = $\leq 2.0\%$ by weight)^[120], 18 cm (ERL, NSW Indian head values, virgin HMX, 99.8% purity)^[120], 26.2 cm (ERL, LANL values, recovered HMX, 100% purity, particle size = 22.45 μ m)^[120], 7.5 Nm (raw HMX, $X_{50.3} = 355$ μ m, 1.923 g cm⁻³)^[123], 7.5 Nm (milled HMX using annular gap ball mill, $X_{50.3} = 0.58$ μ m, 1.951 g cm⁻³)^[123], 6.0 Nm (HMX micronization by PCA process, $X_{50.3} = 7.6$ μ m, 1.939 g cm⁻³)^[123], IS of δ -HMX is independent of crystal size and method of synthesis, and δ -HMX is more sensitive when no grit is on the drop weight (Cady)^[129], δ -HMX has 22% lower drop height cf. β -HMX (type 12A impact machine, 50% probability, Bruceton method)^[129], $H_{50} = 24$ cm (β -HMX, BAM, type 12 tool)^[130], $H_{50} = 22$ cm (γ -HMX, BAM, type 12 tool)^[130], $H_{50} = 26.4$ cm (sm-HMX (submicron-HMX), >99% γ -polymorph, oblong particles,

average particle width ~300 nm, average particle length = 1–2 μm , type 12 machine)^[131], H_{50} = 24.9 cm (standard-HMX (β -HMX), type 12 machine)^[131], H_{50} = 29 cm (2.5 kg mass, type 12 tool)^[133], 9 in (23 mg sample, P.A.)^[152], 60 cm (B.M.)^[152], 30.7 (FEM-HMX)^[171]

$H_{50\%}$, up-down method, 25 mg samples, pressed to 10 kbar to give pellets of 5 mm diameter, 0.8 mm height; grit was fine, very fine or coarse where stated; PC = polycarbonate, PS = polysulfone, PMMA = polymethyl methacrylate, PP = polypropylene^[54]:

Sample (sample + binder)	50% Height (cm)	Sample (sample + binder)	50% Height (cm)
HMX (pure)	29.0 \pm 2.0	HMX + PMMA (coarse)	22.6 \pm 1.0
HMX + PC (fine)	16.0 \pm 1.5	HMX + PP (fine)	24.4 \pm 0.8
HMX + PS (very fine)	15.1 \pm 1.0		

Size density and sensitivity of HMX crystalline particles, C-HMX (fine) = commonly used β -HMX, fine particles, C-HMX (coarse) = commonly used β -HMX, coarse particles, D-HMX (fine) = desensitized β -HMX, fine particles with mean particle size of ~20 μm , D-HMX (coarse) = desensitized β -HMX, coarse particles with mean particle size of ~150 μm ^[56]:

Material	Mean size, d_{50} (μm)	Average crystal ρ @ 20 °C (g/cm ³)	Drop-weight impact tests	
			Exploding probability Hammer: 10 kg Sample: 50 mg Drop height: 25 cm	H_{50} (cm) of go and no go Hammer: 2 kg Sample: 30 mg
C-HMX (fine)	23.1	1.8984 \pm 0.0005	88% (0.69, 0.98) _{0.95}	16.8 \pm 0.1
C-HMX (coarse)	162.4	1.9003 \pm 0.0005	72% (0.51, 0.88) _{0.95}	59.6 \pm 0.1
D-HMX (fine)	19.6	1.9015 \pm 0.0003	24% (0.09, 0.45) _{0.95}	75.7 \pm 0.1
D-HMX (coarse)	148.9	1.9018 \pm 0.0003	60% (0.45, 0.74) _{0.95}	68.8 \pm 0.1

	Fine and coarse HMX fractions (according to UNST/SG/AC.10/11, ρ measured using liquid pycnometry) ^[90] :			
	Sieve fraction (μm)	ρ (g cm^{-3})	IS (Nm) (trial 1/ trial 2)	Comments
	355–425	1.900	15/15	Recryst., stirrer rate = 360 rpm
	106–180	1.895	25/7.5	Recryst., stirrer rate = 450 rpm
	355–425	1.895	20/15	Recryst., stirrer rate = 450 rpm
	355–425	1.895	10/7.5	As-received
	Particle size (d_{50}) (μm) vs. energy of impact sensitivity tests (approx. values) ^[102] : 3 μm /4 Nm, 10/4, 15/5, 105/75, 103/15, 103/20 ^[102] ρ (pycnometry, g cm^{-3}) vs. energy of impact sensitivity tests (J) ^[102] : 1.873 g cm^{-3} /4.5 J, 1.883/4.5, 1.902/5.0, 1.895/6.5, 1.9/9.0, 1.934/9.5 ^[102] H_{50} values (2.5 kg hammer, according to GJB772A-2005 method 601.2) ^[169] :			
	Sample	wt. / %		H_{50} / cm
		α -HMX	β -HMX	
	β -HMX	0	100	44.1
	HMX-I	60	40	34.1
	HMX-II	80	20	30.7
	HMX-III	90	10	28.4
	α -HMX	100	0	26.1
	H_{50} = 79.10 cm (submicron-HMX, median particle diameter = 616 nm) ^[170] , H_{50} = 34.05 cm (raw HMX) ^[170]			
FS [N]	120 ^[3] , 154.4 ^[7] , 152.56 (20 μm) ^[8] , 141.99 (50 μm) ^[8] , 141.70 (100 μm) ^[8] , 142.46 (200 μm) ^[8] , 126.88 (300 μm) ^[8] , 114.12 (400 μm) ^[8] , 154.4 ^[9] , $P_{\text{fr.LL}}$ = 200 MPa ^[19] , $P_{\text{fr.50\%}}$ = 350 MPa ^[19] , Rotary friction test: mean figure of friction (FOF) = 2.5 ^[20] , BAM mean limiting load = 147 ^[20] , mallet friction test: steel on steel = 50%, nylon on steel = 0%, wood on softwood = 0%, wood on hardwood = 0%, wood on Yorkstone = 0% ^[20] , explodes with steel shoe (friction pendulum test) ^[14, 16, 152] , unaffected by fiber shoe (friction pendulum test) ^[14, 16] , 113 (BAM Julius-Peters) ^[50] , 11–17 kg (BAM) ^[51] , 100 psi @ 4 ft/s (ABL) ^[51] , 8.0 kg (Julius-Peters, HMX Klasse-C) ^[60] , 100 Nm (50% value) ^[61] , 50 psi @ 4 ft/s (ABL) ^[67] , Rotter FoF = 2.5 ^[72] , Rotter FoF = 1.5 ^[72] , 147 (BAM, limiting load) ^[72] , 80 (BAM limiting load) ^[72] , 120 (BAM limiting load) ^[72] , 11–17 kg (BAM) ^[80] , 50–100 psi @ 4 ft/s (ABL) ^[80] , 144 ^[88] , 144 (20 °C, 42% rel.			

	<p>humidity, time of sample bead milling = 0 h)^[99], 216 (20 °C, 42% rel. humidity, time of sample bead milling = 1.0 h)^[99], 240 (20 °C, 42% rel. humidity, time of sample bead milling = 5.9 h)^[99], 96 ($d_{50,3}$ = 0.58 μm, ball milled)^[103], 108 ($d_{50,3}$ = 355 μm)^[103], 120 ($d_{50,3}$ = 7.6 μm, particles processed by PCA)^[103], P = 100% (explosion probability, angle of pendulum = 90°, rel. pressure = 3.92 MPa)^[114], 128 (HMX core material, mean particle size = 197 μm)^[117], 160 (pure HMX after 3 h fluidized bed process), mean particle size = 75 μm (abrasion)^[117], 108 (raw HMX, $X_{50,3}$ = 355 μm, 1.923 g cm⁻³)^[123], 96 (milled HMX using annular gap ball mill, $X_{50,3}$ = 0.58 μm, 1.951 g cm⁻³)^[123], 120 (HMX micronization by PCA process, $X_{50,3}$ = 7.6 μm, 1.939 g cm⁻³)^[123], 15.6 kg (50% load, sm-HMX (submicron-HMX), >99% γ-polymorph, oblong particles, average particle width ~300 nm, average particle length = 1–2 μm, BAM)^[131], 11.6 kg (50% load standard-HMX (β-HMX), BAM)^[131], 116 (micro-HMX)^[164], 156 (submicro-HMX)^[164], 183.5 (FEM-HMX)^[171]</p> <p>Wood mallet on stone = 0%^[158], wood mallet on soft wood = 0%^[158], wood mallet on hard wood = 0%^[158]</p> <p>ρ (g cm⁻³, calcd. from X-ray diffraction measurements) vs. pin load (N) of friction tests, approx. values^[102]: 1.885/60, 1.887/80, 1.888/85, 1.888/95, 1.89/110, 1.892/130, 1.879/145^[102]</p> <p>particle size (d_{50}, μm) vs. pin load of friction tests (N) (approx. values)^[102]: 4 μm/80 N, 10/85, 12/108, 104/97, 104/130, 105/145^[102]</p> <p>Test swing angle = 80°, 2.45 MPa pressure, % probability of explosion^[169]:</p> <table><tr><th rowspan="2">Sample</th><th colspan="2">wt./%</th><th rowspan="2">P/%</th></tr><tr><th>α-HMX</th><th>β-HMX</th></tr><tr><td>β-HMX</td><td>0</td><td>100</td><td>86</td></tr><tr><td>HMX-I</td><td>60</td><td>40</td><td>92</td></tr><tr><td>HMX-II</td><td>80</td><td>20</td><td>96</td></tr><tr><td>HMX-III</td><td>90</td><td>10</td><td>98</td></tr><tr><td>α-HMX</td><td>100</td><td>0</td><td>100</td></tr></table>	Sample	wt./%		P /%	α-HMX	β-HMX	β-HMX	0	100	86	HMX-I	60	40	92	HMX-II	80	20	96	HMX-III	90	10	98	α-HMX	100	0	100
Sample	wt./%		P /%																								
	α-HMX	β-HMX																									
β-HMX	0	100	86																								
HMX-I	60	40	92																								
HMX-II	80	20	96																								
HMX-III	90	10	98																								
α-HMX	100	0	100																								
ESD [J]	<p>0.21–0.23 (<100 μm), 2.89^[1, 4], 236.4 mJ^[4], spark sensitivity: 0.2 (brass electrode, 3 mm Pb foil thickness)^[16, 17], 1.03 (brass electrode, 10 mm Pb foil thickness)^[16, 17], 0.12 (steel electrode, 1 mm Pb foil thickness)^[16, 17], 0.87 (steel electrode, 10 mm Pb foil thickness)^[16, 17], 225 ≥ 726 mJ^[50], depends on size^[51], $E_{50\%}$ = 0.25^[67], $E_{50\%}$ = 0.21 ± 0.09 (Bruceton formula)^[69], $E_{50\%}$ = 0.17 ± 0.02 (Bruceton formula)^[69], $E_{50\%}$ = 0.23 (LANL using 0.008 cm Pb foil confinement)^[69], 56–1,800 mJ (old equipment, different particle sizes), >5,600 mJ (medium particle size of 341 μm, new equipment)^[122], energy in capacitors = 182 mJ, spark duration = short^[124], 0.625 (threshold of</p>																										

initiation, sm-HMX (submicron-HMX), >99% γ -polymorph, oblong particles, average particle width ~300 nm, average particle length = 1–2 μm , ABL-ESD machine)^[131], 0.25 (threshold of initiation, standard-HMX (β -HMX), ABL-ESD)^[131], 0.25 (micro-HMX)^[164], 0.625 (submicro-HMX)^[164], 0.1050 (FEM-HMX)^[171], 0.400 (40,000 Voltage, 100 sieve, for zero ignition, 500 MMF capacitance, 0.005" gap setting)^[173]

Data from^[180]:

Material	50% Point energy (J)		
	3-mil foil	10-mil foil	% Expl.
HMX (impact std)	0.23	1.42	23

Heated explosives, HMX (88–63), * = Polystyrene holders, † = Teflon holders^[180]:

T (°C)	50% Point energy (J)		
	3-mil foil	10-mil foil	% Expl.
22	0.26	1.12	75*
75	0.26	1.03	0 [†]
125	0.19	0.80	0 [†]
175	0.12	0.52	25 [†]
200	0.125	0.36	54 [†]

Heated molding powders, * = Polystyrene holders, † = Teflon holders^[180]:

T (°C)	50% Point energy (J)		
	3-mil foil	10-mil foil	% expl.
9,404 (94/3/3, HMX/NC/CEF)			
22	0.42	3.13	0*
75	0.33	3.25	0 [†]
125	0.30	2.50	0 [†]
175	0.24	1.92	25 [†]
LX-04 (85/15, HMX/Viton)			
22	1.04	2.58	38*
75	0.78	2.25	0 [†]
125	0.73	2.10	42 [†]
175	0.65	2.15	31 [†]

N [%]	37.84
$\Omega(\text{CO}_2)$ [%]	–21.61

$T_{\text{phase transition}} [^{\circ}\text{C}]$	<p>193 ($\beta \rightarrow \delta$-), >160–164 ($\alpha \rightarrow \delta$-)[¹⁶], meta exists at 160–164[¹⁶], 102–104.5 ($\beta \rightarrow \alpha$-)[¹⁶], 192 ($\beta \rightarrow \delta$- crystalline phase transition, endo, irrev., DTA @ 2 $^{\circ}\text{C}/\text{min}$)[³⁰], 193–201 ($\alpha \rightarrow \delta$-)[^{30, 35}], 167–183 ($\beta \rightarrow \delta$-)[^{30, 35}], 167–182 ($\gamma \rightarrow \delta$-)[³⁰], 154 ($\beta \rightarrow \gamma$-)[^{30, 35}], 116 ($\alpha \rightarrow \beta$-)[^{30, 35}], 181–193 (DSC, $\beta \rightarrow \delta$-)[⁴¹], 188–194 (DSC, $\alpha \rightarrow \delta$-)[⁴¹], 171–182 ($\gamma \rightarrow \delta$-)[⁴¹],</p> <p>$\beta$-HMX $\xrightarrow{\text{heating} > 102-104.5\text{ }^{\circ}\text{C}}$ α-HMX $\xrightarrow{\text{heating } 160-164\text{ }^{\circ}\text{C}}$ γ-HMX $\xrightarrow{\text{heating} > 160-164\text{ }^{\circ}\text{C}}$ δ-HMX [27]</p> <p>192 (DTA @ 2 $^{\circ}\text{C}/\text{min}$, 1 atm, β-HMX in air, endo, irreversible cryst. phase transition of $\beta \rightarrow \delta$-)[³⁰], 185 ($\beta \rightarrow \delta$- phase transition, endo, DTA)[³⁰], HMX-I is RT stable form[²²], HMX-II is stable form from 115–156 $^{\circ}\text{C}$[²²], HMX-III has only a very narrow stability range @ atmospheric pressure @ 156 $^{\circ}\text{C}$[²²], HMX-IV is stable from ~156 $^{\circ}\text{C}$ to mpt. of 279 $^{\circ}\text{C}$[²²], pure samples of the unstable polymorphs transform to β-HMX @ RT (except in presence of solvent)[⁴¹], ~159 $^{\circ}\text{C}$ $\beta \rightarrow \delta$- (most commonly observed phase transition) [⁴¹], presence of RDX impurities facilitates $\beta \rightarrow \delta$- conversion @ 159 $^{\circ}\text{C}$[⁴¹], no $\beta \rightarrow \delta$- conversion <170 $^{\circ}\text{C}$ if RDX-free HMX[⁴¹], $\beta \rightarrow \delta$- (s) \rightarrow (s) phase transition occurs @ RT if both polymorphs in close contact[⁴¹], δ-HMX can be stored indefinitely without phase transition to β-HMX occurring if pure[⁴¹], $\beta \rightarrow \alpha$- occurs @ 170–190 $^{\circ}\text{C}$[⁴¹], $\alpha \rightarrow \beta$- (for solids) not observed[⁴¹], $\alpha \rightarrow \delta$- >190 $^{\circ}\text{C}$, reverse transition not observed[⁴¹], $\beta \rightarrow \gamma$- not observed[⁴¹], but $\gamma \rightarrow \beta$- occurs @ RT (s)[⁴¹], ~190 (insensitive $\beta \rightarrow$ sensitive δ-, approx. 6.7% volume expansion)[⁶⁵], 192.0 (endo, DSC @ 10 $^{\circ}\text{C}/\text{min}$, $\beta \rightarrow \delta$-, rate constant from $7.2 \times 10^{-4}\text{ s}^{-1}$ @ 178 $^{\circ}\text{C}$ to $2.6 \times 10^{-3}\text{ s}^{-1}$ @ 183 $^{\circ}\text{C}$, $E_a = 416.6\text{ kJ mol}^{-1}$)[⁶⁵], 190–195</p> <p>($\beta \rightarrow \delta$- occurring, 24.9% of HMX is δ- @ 195 $^{\circ}\text{C}$, only 5% β- remained @ 210 $^{\circ}\text{C}$, 98.5% δ- on cooling back to 30 $^{\circ}\text{C}$, in situ XRD, Rietveld refinement)[⁶⁵], $\varepsilon \rightarrow \delta$- occurs via intermediate formation of β-HMX[¹⁰⁰], heating a ε-HMX single crystal to 170 $^{\circ}\text{C}$ followed by rapid cooling results in formation of a single crystal of β-HMX[¹⁰⁰], heating single crystal of ε-HMX to 200 $^{\circ}\text{C}$ results in formation of polycrystalline aggregate of δ-HMX[¹⁰⁰], $\varepsilon \rightarrow \beta$- transformation occurs immediately after grinding ε-HMX crystals in agate mortar[¹⁰⁰], no phase transition between ambient temperature and 280 $^{\circ}\text{C}$ (sm-HMX (submicron-HMX), >99% γ-polymorph, oblong particles, average particle width ~300 nm, average particle length = 1–2 μm, DSC @ 1 K/min up to 200 $^{\circ}\text{C}$, then 5 K/min)[¹³¹], β-HMX is stable to ~102–104.5 $^{\circ}\text{C}$ ($\beta \rightarrow \alpha$-)[¹⁶], metastable γ-form exists @ 160–164 $^{\circ}\text{C}$[¹⁶], δ- form exists >160–164 $^{\circ}\text{C}$[¹⁶], the four different HMX polymorphs can be prepared by precipitation from different solvents[¹⁶], metastable @ RT (α-HMX)[¹⁵⁰], stable @ RT (β-HMX)[¹⁵⁰], metastable @ RT (γ-HMX)[¹⁵⁰], labile @ RT (δ-HMX)[¹⁵⁰]</p> <p>HMX phase transition T from DSC[⁴¹]: $\beta \rightarrow \delta$- @ 454–466 K (181–193 $^{\circ}\text{C}$)[⁴¹], $\alpha \rightarrow \delta$- @ 461–467 K (188–194 $^{\circ}\text{C}$)[⁴¹], $\gamma \rightarrow \delta$- @ 444–455 K (171–182 $^{\circ}\text{C}$)[⁴¹], no phase transition to a plastically crystalline phase @ high T[⁴¹]</p> <p>196.31 ($\beta \rightarrow \delta$-, LC-HMX, DSC @ 1 $^{\circ}\text{C}/\text{min}$, 1 mg sample, N_2 atm.)[⁵⁵], 193.96 ($\beta \rightarrow \delta$-, FC-HMX, DSC @ 1 $^{\circ}\text{C}/\text{min}$, 1 mg sample, N_2 atm.)[⁵⁵], 202.33 ($\beta \rightarrow \delta$-, LD-HMX, DSC @ 1 $^{\circ}\text{C}/\text{min}$, 1 mg sample, N_2 atm.)[⁵⁵], 203.81 ($\beta \rightarrow \delta$-, FD-HMX, DSC @ 1 $^{\circ}\text{C}/\text{min}$, 1 mg sample, N_2 atm.)[⁵⁵], 180 ($\beta \rightarrow \delta$-, DSC @ 5 $^{\circ}\text{C}/\text{min}$, 5 mg sample)[⁶⁰]</p>
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Summary of phase transition temperatures (°C) in the literature cited in^[68]:

Transition	Goetz & Brill (slow heating)	Goetz and Brill (rapid heating)	McCrone	Fedoroff	Orlova et al.	Firsich	Achuthan & Jose
$\beta \rightarrow \alpha$	—	175	115	102	115	102	115
$\beta \rightarrow \delta$	142	175	—	—	—	—	—
$\alpha \rightarrow \gamma$	—	—	156	160	156	160	—
$\alpha \rightarrow \delta$	147	185	—	—	—	—	—
$\gamma \rightarrow \delta$	205	170	156	164	271	164	—

β -HMX obtained by crystallization from acetone solution^[100], γ -HMX by dissolving β -HMX under moderate heating in cyclohexanone then adding the soln. to dichloroethane and filtration of γ -HMX crystals^[100], ε -HMX obtained as coproduct of $\beta \rightarrow \delta$ transformation in presence of cyclohexanone near bpt. of solvent (ca. 152–153 °C)^[100], spindle-shaped δ -HMX crystals change into fine-grained opaque aggregates of β -HMX days after crystallization^[100], heat effect of transitions^[100]: -1.88 kcal/mol ($\alpha \rightarrow \delta$)^[100], -2.14 kcal/mol $\beta \rightarrow \delta$.^[100], -1.10 kcal/mol $\gamma \rightarrow \delta$.^[100], -2.21 kcal/mol $\alpha \rightarrow \delta$.^[100]

388.5 K ($\beta \rightarrow \alpha$, $\Delta H = 1.9$ kJ/mol)^[78], 439.0 K ($\alpha \rightarrow \delta$, $\Delta H = 7.95$ kJ/mol)^[78]

$\beta \rightarrow \delta$ phase transition T , (<74 μ m particle size, endo) @ various heating rates, open pan, using DSC^[128]:

Heating rate (°C/min)	T_{onset} (°C)	T_{peak} (°C)	ΔH (J/g)
10	192.2 \pm 0.6	196.2 \pm 0.6	30.6
15	194.6 \pm 0.1	199.5 \pm 0.8	29.4
20	195.5 \pm 0.5	201.4 \pm 0.7	30.1
25	196.9 \pm 0.9	202.6 \pm 0.6	31.1

$\beta \rightarrow \delta$ phase transition T @ 15 °C/min, 2.5 mg sample, open pan, various particle sizes, using DSC^[128]:

Particle size (μ m)	T_{onset} (°C)	T_{peak} (°C)	ΔH (J/g)
>354	181.0 \pm 0.6	186.5 \pm 0.6	27.8 \pm 0.1
177–354	178.6 \pm 0.6	191.4 \pm 2.1	27.4 \pm 0.3
125–177	188.9 \pm 0.8	194.9 \pm 0.3	28.2 \pm 0.4
74–125	194.7 \pm 0.5	199.6 \pm 0.3	26.8 \pm 0.9
<74	193.3 \pm 0.5	200.5 \pm 0.7	29.6 \pm 2.7

158–190 (range of values for 0.05–10 °C/s heating rates, $\beta \rightarrow \delta$ phase transition)^[129], α -HMX stable @ 103–162 °C^[130], δ -HMX stable from 182 °C \rightarrow mpt.^[130], γ -HMX metastable with respect to other polymorphs^[130], $\gamma \rightarrow \beta$ occurs @ 85 °C and polar solvent (e.g. H₂O)^[130]

Fig. 14 data from^[130]:

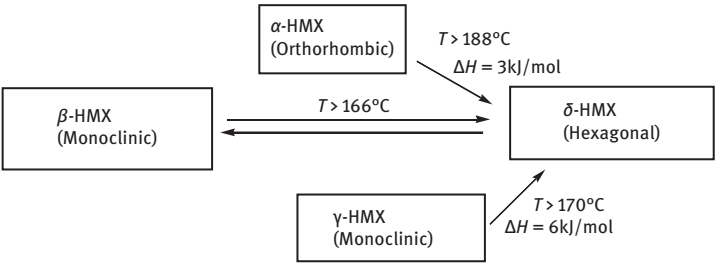


Fig. 14: Interconversion of different polymorphs of HMX^[130].

Arrhenius data for the three thermally induced solid-phase transformation of HMX at 1 atm.^[130]:

HMX phase transition	E_a (kJ/mol)	Log A (Arrhenius factor)	T (°C)
$\beta \rightarrow \delta$ -	204 ± 14	19.9 ± 1	166–294
$\alpha \rightarrow \delta$ -	208 ± 18	19.9 ± 2	188–200
$\gamma \rightarrow \delta$ -	219 ± 20	21.8 ± 2	171–185

Pouring acetone or acetonitrile soln. of β -HMX into cold H₂O (10 °C) precipitates fluffy powder of γ -HMX^[130], heating γ -HMX in H₂O results in conversion to crystalline β -HMX^[130], α -HMX, β -HMX and γ -HMX are stable up to 275 °C (TGA/DTA)^[130], pressing pellets of nano- γ -HMX causes conversion to β -HMX^[130], 180–190 ($\beta \rightarrow \delta$ -, solid state, @ 10 °C/min, STA, exact value depends on heating rate)^[130]

180 (weak endo, DSC @ 5 °C/min, β - (monoclinic) \rightarrow δ - (hexagonal), 0.5–2.5 mg sample, Al pan with perforated cover, N₂)^[132], 190 (weak endo, DSC @ 20 °C/min, β - (monoclinic) \rightarrow δ - (hexagonal), 0.5–2.5 mg sample, Al pan with perforated cover, N₂)^[132]

β -HMX decomposes @ elevated T in the pressure range 0.2–6.5 GPa^[135], but $\beta \rightarrow \delta$ - occurs @ 453–493 K @ pressures <0.2 GPa^[135]

	<p>193–201 ($\alpha \rightarrow \delta$)^[162], 167–183 ($\beta \rightarrow \gamma$)^[162], 167–182 ($\gamma \rightarrow \delta$)^[162], 167–183 ($\beta \rightarrow \delta$)^[174], 154 ($\beta \rightarrow \gamma$)^[174], 102–104 ($\beta \rightarrow \gamma$)^[174], 193–201 ($\alpha \rightarrow \delta$)^[174], 116 ($\alpha \rightarrow \beta$)^[174], metastable ($\alpha \rightarrow \gamma$)^[174], 160–164 ($\alpha \rightarrow \delta$)^[174], 167–182 ($\gamma \rightarrow \delta$)^[174]</p> <p>Data from^[17]:</p> <table><tr><th rowspan="2">Type</th><th rowspan="2">T (°C)</th><th colspan="2">Latent heat</th></tr><tr><th>cal/g</th><th>kcal/mol</th></tr><tr><td colspan="2">Solid–solid</td><td></td><td></td></tr><tr><td>β to α</td><td>102–104</td><td>2.0</td><td>0.6</td></tr><tr><td>α to γ</td><td>Metastable</td><td>–</td><td>–</td></tr><tr><td>α to δ</td><td>160–164</td><td>7.8</td><td>2.3</td></tr></table>	Type	T (°C)	Latent heat		cal/g	kcal/mol	Solid–solid				β to α	102–104	2.0	0.6	α to γ	Metastable	–	–	α to δ	160–164	7.8	2.3
Type	T (°C)			Latent heat																			
		cal/g	kcal/mol																				
Solid–solid																							
β to α	102–104	2.0	0.6																				
α to γ	Metastable	–	–																				
α to δ	160–164	7.8	2.3																				
$T_{\text{mpt.}}$ [°C]	285 ^[12, 16] , 246 ^[12, 137, 146] , 276 ^[12] , 273 ^[12, 36, 86] , 273 (capillary method) ^[14] , 280 (Koffler microhot stage) ^[14] , 256–257 (α -) ^[17, 174] , 246–247 (β -) ^[17, 174] , 279–280 (γ -) ^[17, 174] , 280–281 (δ -) ^[17] , 280 ^[39] , 282 ^[41] , 276–280 (with dec.) ^[27] , 226–227 ^[25] , 280 (dec.) ^[36, 50] , 271.8 (dec., Mettler mpt. apparatus, @ 1 K/min beginning 10 K beneath the mpt.) ^[162] , 553.15 K ^[172] , 280–281.5 (γ -HMX, form III) ^[174]																						
$T_{\text{b.p.}}$ [°C]	dec. ^[52] , 744 ± 37 K (est. by estimating the vapor pressure over liq. HMX and extrapolating to atmospheric pressure) ^[73] , 800 ± 4 K (est. <i>Lyman et al.</i>) ^[80] , 709.5 K (T_{nbp} , est., Stein-Brown method) ^[172]																						
$T_{\text{dec.}}$ [°C]	276 (DSC @ 5 °C/min), 200 ^[12] , 509 K (DTA) ^[6] , 282 (α -HMX, DTA @ 10 °C/min), 276 (violent dec. of δ -HMX, DTA @ 2 °C/min.) ^[30] , 244 (DSC @ 20 °C/min, exotherm peak max.) ^[39] , 280 (dec.) ^[36] , 279 (violent dec. exotherm, DTA) ^[30] , 276 (violent dec. of δ -HMX, DTA @ 2 °C/min of β -HMX) ^[30] , 271 (onset, exo), 276 (exo peak max.) (DSC @ 5 °C/min, 5 mg sample) ^[60] , 240 (TG onset) ^[61] , 250 (exo reaction) ^[61] , 284.8 (exo, enthalpy = 1,624 J g ⁻¹) ^[65] , 264 (dec. onset) ^[93] , 534 K (pyrolytic dec./deflagration) ^[92] , 284.6 (PDSC @ 10 °C/min @ 3 MPa) ^[93] , 283.2 (PDSC @ 10 °C/min @ 1 MPa) ^[93] , 284.0 (PDSC @ 10 °C/min @ 0.1 MPa) ^[93] , 275 (exo, DTA) ^[106] , 279.8 (onset), 283 (peak max) (DSC, virgin HMX, 99.8% purity) ^[120] , 251 (onset), 283 (peak max) (DSC, recovered HMX, 100% purity) ^[120] , 278 (β -HMX, STA @ 5 °C/min) ^[130] , 285 (γ -HMX, STA @ 5 °C/min) ^[130] , 281 (sm-HMX (submicron-HMX), >99% γ -polymorph, oblong particles, average particle width ~300 nm, average particle length = 1–2 μm , DSC @ 1 K/min from ambient temperature to 200 °C then 5 K/min, 1 mg sample crimped in Al pans) ^[131]																						
	Extent of β -HMX dec. (mole fraction) vs. time (s) for the thermal decomposition of β -HMX @ 3.6 GPa and various temperatures ^[135] :																						

Time (s)	@ 568 K	@ 563 K	@ 558 K	@ 553 K
~100	~0.4			
~200	~0.82			
~500		~0.32		
~800		~0.68	~0.24	
~1,300			~0.38	~1.7
~2,000			~0.55	
~2,500			~0.75	
~2,800			~0.82	~0.4
~3,000			~0.92	
~3,800				~0.54
~4,300				~0.62
~5,300				~0.72

Heating rate of 8 °C/min: $T_{\text{idb}} = 264.9^{[40]}$, $T_w = 267.6^{[40]}$, $T_{\text{max}} = 272.0^{[40]}$

Heating rate of 16 °C/min: $T_{\text{idb}} = 278.3^{[40]}$, $T_w = 284.7^{[40]}$, $T_{\text{max}} = 290.9^{[40]}$,
 $T_{\text{cr}} = 253\text{--}255^{[40]}$

Data from^[169]:

Sample	β (°C/min)	T_p (°C)
β -HMX	5	283.3
β -HMX	10	287.3
β -HMX	15	292.0
β -HMX	20	297.0
HMX-I	5	282.6
HMX-I	10	286.6
HMX-I	15	291.6
HMX-I	20	296.6
α -HMX	5	282.0
α -HMX	10	286.4
α -HMX	15	291.4
α -HMX	20	296.4

280.62 (exo peak max., raw HMX, DSC @ 5 °C/min)^[170], 284.30 (exo peak max., raw HMX, DSC @ 10 °C/min)^[170], 289.05 (exo peak max., raw HMX, DSC

	@ 20 °C/min) ^[170] , 281.26 (exo peak max, submicron-HMX, median particle size = 616 nm, DSC @ 5 °C/min) ^[170] , 285.12 (exo peak max, submicron-HMX, median particle size = 616 nm,, DSC @ 10 °C/min) ^[170] , 290.44 (exo peak max, submicron-HMX, median particle size = 616 nm, DSC @ 20 °C/min) ^[170]																									
ρ [g cm ⁻³]	<p>1.962 (@ 20 K), 1.905 (TMD @ 25 °C)^[17], 1.90^[27, 146], 1.903 (@ 25 °C)^[25], 1.886 (@ 298 K, gas pycnometer), 1.899^[2], 1.90 (crystal)^[14], 1.903 (β-crystal)^[16], 1.82 (α-crystal)^[16], 1.76 (γ-crystal)^[16, 41], 1.80 (δ-HMX)^[41], 1.902^[12], 1.91 (β-HMX)^[50], 1.894^[63], 1.904^[93], 1.839 (α-HMX)^[100], 1.902 (β-HMX)^[100], 1.82 (γ-HMX)^[100], 1.763 (δ-HMX)^[100], 1.919 (ε-HMX)^[100], 1.90 (β-HMX)^[134], 1.87 (crystals)^[139], 1.905 (TMD)^[16], 1.89 (nominal)^[16], 1.905 (@ TMD)^[142], 1.905^[158, 167], 1.91 (FEM-HMX)^[171], 1.893 (β-HMX, form I, X-ray)^[174], 1.902 (β-HMX, form I, X-ray)^[174], 1.839 (α-HMX, form II, X-ray)^[174], 1.759 (δ-HMX, form IV, X-ray)^[174], 1.78 (γ-HMX, form III, X-ray)^[174], 1.82 (γ-HMX, form III, X-ray)^[174]</p> <p>Purity and particle density of HMX particles^[55]:</p> <table><tr><th>Sample</th><th>LD-HMX</th><th>LC-HMX</th><th>FD-HMX</th><th>FC-HMX</th></tr><tr><td>Purity</td><td>99.7 ± 0.1</td><td>99.3 ± 0.1</td><td>99.6 ± 0.1</td><td>99.2 ± 0.1</td></tr><tr><td>Mean ρ (g cm⁻³)</td><td>1.9018</td><td>1.9003</td><td>1.9016</td><td>1.8984</td></tr><tr><td>% TMD (based on TMD = 1.903 g cm⁻³)</td><td>99.94</td><td>99.86</td><td>99.93</td><td>99.76</td></tr><tr><td>ρ Distribution (g cm⁻³)</td><td>1.9012– 1.9020</td><td>1.8973– 1.9018</td><td>1.9010– 1.9019</td><td>1.8970– 1.8993</td></tr></table> <p>1.8806 (0.0005) (cryst., type B, class 1, Dyno Nobel, Norway)^[98], 1.8891 (0.0009) (cryst., type B, 10–15 μm, Dyno Nobel, Norway)^[98], 1.8974 (0.0010) (cryst., recryst. from PC (propylene carbonate))^[98], 1.9016 (0.0003) (cryst., recryst. from γ-BL = γ-butyrolactone)^[98], 1.9002 (nonsieved reference HMX, class 6, d_{10} = 71.50 μm, d_{50} = 130.33 μm, d_{90} = 208.53 μm, Dyno Nobel)^[103], 1.895 (RS-HMX, recryst. from propylene carbonate, d_{10} = 45.78 μm, d_{50} = 104.45 μm, d_{90} = 175.25 μm, ICT)^[103], 1.8735 (Fine HMX, HMX comminuted with annular gap mill, d_{10} = 0.92 μm, d_{50} = 1.64 μm, d_{90} = 31.71 μm, ICT)^[103], 1.9330 (HMX comminuted with annular gap mill, d_{10} = 0.92 μm, d_{50} = 1.64 μm, d_{90} = 3.07 μm, ICT)^[103]</p> <p>Effect of bead milling (time of milling (h)/ρ (g cm⁻³))^[99]: 0/1.8931^[99], 1.0/1.8976^[99], 5.9/1.8988^[99]</p> <p>Average particle ρ (g cm⁻³)/ particle ρ distribution (g cm⁻³)^[105]: 1.898/1.894–1.900 (standard HMX, class 1), 1.898/1.897–1.899 (standard HMX, class 5), 1.901(1.900–1.902) (RS-HMX)^[105]</p>	Sample	LD-HMX	LC-HMX	FD-HMX	FC-HMX	Purity	99.7 ± 0.1	99.3 ± 0.1	99.6 ± 0.1	99.2 ± 0.1	Mean ρ (g cm ⁻³)	1.9018	1.9003	1.9016	1.8984	% TMD (based on TMD = 1.903 g cm ⁻³)	99.94	99.86	99.93	99.76	ρ Distribution (g cm ⁻³)	1.9012– 1.9020	1.8973– 1.9018	1.9010– 1.9019	1.8970– 1.8993
Sample	LD-HMX	LC-HMX	FD-HMX	FC-HMX																						
Purity	99.7 ± 0.1	99.3 ± 0.1	99.6 ± 0.1	99.2 ± 0.1																						
Mean ρ (g cm ⁻³)	1.9018	1.9003	1.9016	1.8984																						
% TMD (based on TMD = 1.903 g cm ⁻³)	99.94	99.86	99.93	99.76																						
ρ Distribution (g cm ⁻³)	1.9012– 1.9020	1.8973– 1.9018	1.9010– 1.9019	1.8970– 1.8993																						

	1.8806 ± 0.0005 (crystal, HMX type B, class 1, 0.67% RDX impurity, fluid pycnometer) ^[115] , 1.8891 ± 0.0009 (crystal, HMX type B, 10–15 µm, 0.22% RDX impurity, fluid pycnometer) ^[115] , 1.8974 ± 0.0010 (crystal, HMX recrystallized from PC, 0.04% RDX impurity, fluid pycnometer) ^[115] , 1.9016 ± 0.0003 (crystal, HMX recrystallized from butyrolactone, 0.02% RDX impurity, fluid pycnometer) ^[115] , 1.91 (β-HMX) ^[130] , 1.82 (γ-HMX) ^[130] , sp. gr. = 1.96 (α-HMX) ^[150] , sp. gr. = 1.87 (β-HMX) ^[150] , sp. gr. = 1.82 (γ-HMX) ^[150] , sp. gr. = 1.77 (δ-HMX) ^[150] Data from ^[17] : <table><tr><th rowspan="2">Method of determination</th><th rowspan="2">State</th><th colspan="4">Density (g/cm³)</th></tr><tr><th>α</th><th>β</th><th>γ</th><th>δ</th></tr><tr><td>X-ray</td><td>Solid</td><td>1.838</td><td>1.902</td><td>1.78</td><td>1.786</td></tr><tr><td>Direct measurement</td><td>Solid</td><td>1.84</td><td>1.905</td><td>1.76</td><td>1.80</td></tr></table>				Method of determination	State	Density (g/cm ³)				α	β	γ	δ	X-ray	Solid	1.838	1.902	1.78	1.786	Direct measurement	Solid	1.84	1.905	1.76	1.80
Method of determination	State	Density (g/cm ³)																								
		α	β	γ	δ																					
X-ray	Solid	1.838	1.902	1.78	1.786																					
Direct measurement	Solid	1.84	1.905	1.76	1.80																					
Heat of formation	11.3–17.93 kcal per mol ^[16] , 11.3 kcal mol ⁻¹ (ΔH ^o _f) ^[17] , 17.92 kcal mol ⁻¹ (ΔH _f , crystal @ 25 °C) ^[25] , –17.1 kcal mol ⁻¹ ^[27] , 11.3 kcal/mol ^[112] , 17.93 kcal/mol ^[112] , 255.2 kJ/kg ^[2] , 60.0 kcal/kg (enthalpy of form.) ^[85] , 87.8 kJ/mol (enthalpy of form.) ^[93] , 24.5 kcal/mol (ΔH _f (s)) ^[63] , 84 kJ/mol (enthalpy of form.) ^[50] , 17.9 kcal/mol (ΔH ^o _f) ^[57] , 92.8 kJ/mol (ΔH _f) ^[64] , 75.02 kJ/mol ^[142] , –60.5 kcal/kg ^[28] , –60.5 cal/g ^[14] , 21 ± 0.66 kcal/mol (ΔH _f ²⁹⁸ , based on exptl. ΔQ _c value) ^[162] , 75 (no units given) ^[171] , 17.9 kcal/mol ^[183] , –11.90 kcal/mol (–ΔH _f (heat of form. @ standard conditions)) ^[184]																									
Heat of combustion	667.4 kcal/mol ^[27] , 2,362 kcal/kg ^[28] , 2362 cal/g ^[14] , heat of comb. = 660.7–667.4 kcal/mol ^[16] , ΔH _c = –9,330 kJ/kg ^[61] , ΔQ _c = 674 ± 0.66 kcal/mol (exptl.) ^[162] , ΔH ^o _c = –660.7 kcal/mol ^[17] Exptl. heat of combustion data ^[184] : <table><tr><th>–ΔU_{B/M} (cal/g)</th><th>–ΔU_B (kcal/mol)</th><th>–ΔU_R (kcal/mol @ 1 atm and constant vol.)</th><th>–ΔH_R (kcal/mol @ 1 atm. and constant pressure)</th></tr><tr><td>2,254.93 ± 0.86</td><td>667.84</td><td>666.61</td><td>663.06</td></tr></table>				–ΔU _{B/M} (cal/g)	–ΔU _B (kcal/mol)	–ΔU _R (kcal/mol @ 1 atm and constant vol.)	–ΔH _R (kcal/mol @ 1 atm. and constant pressure)	2,254.93 ± 0.86	667.84	666.61	663.06														
–ΔU _{B/M} (cal/g)	–ΔU _B (kcal/mol)	–ΔU _R (kcal/mol @ 1 atm and constant vol.)	–ΔH _R (kcal/mol @ 1 atm. and constant pressure)																							
2,254.93 ± 0.86	667.84	666.61	663.06																							
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.																							
–Δ _{ex} U ^o [kJ kg ⁻¹]	5,837	1,356 cal/g [H ₂ O (l)] (calcd.) ^[27] 1,222 cal/g [H ₂ O (g)] (calcd.) ^[27]	1,356 cal/g ^[14] 1.62 kcal/g [H ₂ O (l)] ^[16]																							

		<p>1,365 kcal/kg^[28]</p> <p>1.50 kcal/g (Q_{\max}, calcd.)^[63]</p> <p>5,668^[93]</p> <p>1,256 kcal/kg (@ 1.300 g cm⁻³, calcd.) [H₂O vapor]^[85]</p> <p>1,301 kcal/kg (@ 1.800 g cm⁻³, calcd.) [H₂O vapor]^[85]</p> <p>1,222 cal/g (calcd.)^[149]</p> <p>Heat of det., = -6.78 MJ/kg^[167]</p>	<p>7.48 kcal/g [H₂O (g)]^[16]</p> <p>1,356 cal/g [H₂O (l)]^[27]</p> <p>1,222 cal/g [H₂O (g)]^[27]</p> <p>5,558 J/g (heat of explosion)^[60]</p> <p>6,192 (@ 1.89 g cm⁻³, heat of detonation, heavily confined charge) [H₂O (l)]^[81]</p> <p>5,719 (@ 1.89 g cm⁻³, heat of detonation, heavily confined charge) [H₂O (g)]^[81]</p> <p>5,527 (@ 1.20 g cm⁻³, heat of detonation, heavily confined charge) [H₂O (l)]^[81]</p> <p>5,116 (@ 1.20 g cm⁻³, heat of detonation, heavily confined charge) [H₂O (g)]^[81]</p> <p>5,808 J/g (@ 1.894 g cm⁻³, det. energy, cylinder test)^[81]</p> <p>5,387 J/g (@ 1.188 g cm⁻³, det. energy, cylinder test)^[81]</p> <p>1,210 kcal/kg (@ 1.300 g cm⁻³) [H₂O vapor]^[85]</p> <p>1,300 kcal/kg (@ 1.800 g cm⁻³) [H₂O vapor]^[85]</p> <p>1,340 kcal/kg (@ 1.81 g cm⁻³, Q_{\exp})^[126]</p> <p>2,580 cal/cm³ (voidless, volumetric heat of explosion)^[152]</p> <p>2,070 cal/cm³ (pressed @ 10,000 psi, volumetric heat of explosion)^[152]</p>
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T_{ex} [K]	3,702	<p>3,689 (@ 1.902 g cm⁻³, calcd.)^[57]</p> <p>4,045 (@ 1.90 g cm⁻³, $\Delta H_f = 17.9$ kcal/mol, calcd. BKWC, THEOSTAR-T)^[112]</p> <p>3,192 (@ 1.90 g cm⁻³, $\Delta H_f = 17.9$ kcal/mol, calcd. BKWR, THEOSTAR-T)^[112]</p> <p>3,250 (@ 100% TMD, calcd., CHEETAH-6)^[119]</p> <p>2,364 (@ 1.90 g cm⁻³, $\Delta H_f^0 = 613.9$ kJ/kg, calcd., FORTRAN BKW)^[143]</p> <p>3,514 (@ 1.905 g cm⁻³, $\Delta H_f = 75$ kJ/mol, calcd., JAGUAR)^[163]</p> <p>3,090 (@ 1.89 g cm⁻³, calcd. BKWR)^[183]</p> <p>3,470 (@ 1.60 g cm⁻³, calcd. BKWR)^[183]</p> <p>3,680 (@ 1.40 g cm⁻³, calcd. BKWR)^[183]</p> <p>3,830 (@ 1.20 g cm⁻³, calcd. BKWR)^[183]</p> <p>3,900 (@ 1.00 g cm⁻³, calcd. BKWR)^[183]</p> <p>4,000 (@ 0.75 g cm⁻³, calcd. BKWR)^[183]</p> <p>4,070 (@ 1.89 g cm⁻³, calcd. BKWS)^[183]</p> <p>4,270 (@ 1.60 g cm⁻³, calcd. BKWS)^[183]</p>	<p>2,364 (@ 1.90 g cm⁻³)^[12]</p> <p>4,300 (@ 1.60 g cm⁻³)^[183]</p>
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		<p>4,380 (@ 1.40 g cm⁻³, calcd. BKWS)^[183]</p> <p>4,450 (@ 1.20 g cm⁻³, calcd. BKWS)^[183]</p> <p>4,480 (@ 1.00 g cm⁻³, calcd. BKWS)^[183]</p> <p>4,440 (@ 0.75 g cm⁻³, calcd. BKWS)^[183]</p>	
<i>p</i> _{C-J} [kbar]	381	<p>385 (calcd., CHEETAH 2.0)^[5]</p> <p>323 (@ 1.77 g cm⁻³, calcd., thermochem.)^[46]</p> <p>393.0 (@ 1.9 g cm⁻³, calcd., thermochem.)^[46]</p> <p>388 GPa (@ 1.90 g cm⁻³ (TMD), calcd., R-P method)^[49]</p> <p>28.0 GPa (@ 1.63 g cm⁻³)^[37]</p> <p>364.0 (@ 1.902 g cm⁻³, calcd.)^[57]</p> <p>381 (@ 1.894 g cm⁻³, calcd.)^[63]</p> <p>376 (@ 1.90 g cm⁻³, Δ<i>H</i>_f = 17.9 kcal/mol, calcd. BKWC, THEOSTAR-T)^[112]</p> <p>399 (@ 1.90 g cm⁻³, Δ<i>H</i>_f = 17.9 kcal/mol, calcd. BKWR, THEOSTAR-T)^[112]</p> <p>367 (@ 100% TMD, calcd., Cheetah-6)^[119]</p> <p>39.5 GPa (@ 1.90 g cm⁻³, Δ<i>H</i>_f⁰ = 613.9 kJ/kg, calcd., FORTRAN BKW)^[143]</p>	<p>389.8 (@ 1.90 g cm⁻³)^[12]</p> <p>5.20 GPa (@ 0.70 g cm⁻³)^[37]</p> <p>28.0 GPa (@ 1.63 g cm⁻³)^[37]</p> <p>316.5 (@ 1.77 g cm⁻³)^[46]</p> <p>376.3 (@ 1.9 g cm⁻³)^[46]</p> <p>5.20 GPa (@ 0.70 g cm⁻³)^[37]</p> <p>28.0 GPa (@ 1.63 g cm⁻³)^[37]</p> <p>40.5 GPa (@ 1.894 g cm⁻³)^[81]</p> <p>15.5 GPa (@ 1.188 g cm⁻³)^[81]</p> <p>42.0 GPa (@ 1.891 g cm⁻³, cylinder test results)^[111]</p> <p>39.3 GPa (@ 1.90 g cm⁻³)^[143]</p> <p>40.5 GPa (@ 1.894 g cm⁻³)^[144]</p> <p>15.5 GPa (@ 1.188 g cm⁻³)^[144]</p> <p>414 cal/cm³ (voidless)^[152]</p> <p>261 cal/cm³ (pressed @ 10,000 psi)^[152]</p> <p>390 (@ 1.89 g cm⁻³)^[183]</p> <p>280 (@ 1.60 g cm⁻³)^[183]</p>

		<p>37.19 GPa (calcd., Cheetah 7.0)^[171]</p> <p>38.7 GPa (@ 1.905 g cm⁻³, $\Delta H_f = 75$ kJ/mol, calcd., JAGUAR)^[163]</p> <p>405 (@ 1.89 g cm⁻³, calcd. BKWR)^[183]</p> <p>281 (@ 1.60 g cm⁻³, calcd. BKWR)^[183]</p> <p>213 (@ 1.40 g cm⁻³, calcd. BKWR)^[183]</p> <p>160 (@ 1.20 g cm⁻³, calcd. BKWR)^[183]</p> <p>117 (@ 1.00 g cm⁻³, calcd. BKWR)^[183]</p> <p>69 (@ 0.75 g cm⁻³, calcd. BKWR)^[183]</p> <p>374 (@ 1.89 g cm⁻³, calcd. BKWS)^[183]</p> <p>259 (@ 1.60 g cm⁻³, calcd. BKWS)^[183]</p> <p>199 (@ 1.40 g cm⁻³, calcd. BKWS)^[183]</p> <p>151 (@ 1.20 g cm⁻³, calcd. BKWS)^[183]</p> <p>110 (@ 1.00 g cm⁻³, calcd. BKWS)^[183]</p> <p>64 (@ 0.75 g cm⁻³, calcd. BKWS)^[183]</p>	<p>210 (@ 1.40 g cm⁻³)^[183]</p> <p>160 (@ 1.20 g cm⁻³)^[183]</p> <p>110 (@ 1.00 g cm⁻³)^[183]</p> <p>60 (@ 0.75 g cm⁻³)^[183]</p>
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VoD [m s ⁻¹]	9,286	9,224 (@ 1.89 g cm ⁻³ , calcd. CHEETAH 2.0) ^[5] 9,150 (@ 1.90 g cm ⁻³ , calcd., K-J) ^[21] 8,773 (@ 1.81 g cm ⁻³) ^[34] 9,110 (@ 1.89 g cm ⁻³) ^[48] 8,500 (@ 1.77 g cm ⁻³ , calcd., thermochem.) ^[46] 9,100 (@ 1.9 g cm ⁻³ , calcd., thermochem.) ^[46] 9,050 (@ 1.90 g cm ⁻³ (TMD), calcd., R-P method) ^[49] 9,230 (@ 1.90 g cm ⁻³ (TMD), calcd., <i>Aizenshtadt</i>) ^[49] 9,120 (@ 1.90 g cm ⁻³ (TMD), calcd., K-J) ^[49] 9,250 (@ 1.902 g cm ⁻³ , calcd.) ^[57] 9,130 (@ 1.894 g cm ⁻³ , calcd.) ^[63] 6,040 (@ 1 g cm ⁻³ , calcd., Kamlet method) ^[87] 8,090 (@ 1.6 g cm ⁻³ , calcd., Kamlet method) ^[87] 5,530 (@ 1 g cm ⁻³ , calcd., Urizar method) ^[87] 7,940 (@ 1.6 g cm ⁻³ , calcd., Urizar method) ^[87] 9,540 (@ 1.90 g cm ⁻³ , $\Delta H_f = 17.9$ kcal/ mol, calcd. BKWC, THEOSTAR-T) ^[112]	9,100 ^[3] 9,110 (@ 1.89 g cm ⁻³) ^[10–12, 16, 17, 21] 7,910 (@ 1.6 g cm ⁻³) ^[10] 7,300 (@ 1.4 g cm ⁻³) ^[10] 6,580 (@ 1.2 g cm ⁻³) ^[10] 5,800 (@ 1.0 g cm ⁻³) ^[10] 4,880 (@ 0.75 g cm ⁻³) ^[10] 9,124 (@ 1.84 g cm ⁻³) ^[14, 26, 27] 8,773 (@ 1.81 g cm ⁻³) ^[34] 5,450 (@ 0.85 g cm ⁻³) ^[37] 8,340 (@ 1.68 g cm ⁻³) ^[37] 9,110 (@ 1.9 g cm ⁻³) ^[37] 4,390 (@ 0.70 g cm ⁻³) ^[37] 7,870 (@ 1.63 g cm ⁻³) ^[37] 1,160 (@ 1.1 g cm ⁻³ , <44 micron particle size, detonated high order @ 4,000 V level) ^[30] 5,450 (@ 0.85 g cm ⁻³) ^[37] 8,340 (@ 1.68 g cm ⁻³) ^[37] 9,110 (@ 1.9 g cm ⁻³) ^[37] 4,390 (@ 0.70 g cm ⁻³) ^[37] 8,458 (@ 1.77 g cm ⁻³) ^[46] 8,919 (@ 1.9 g cm ⁻³) ^[46] 9,110 (@ 1.89 g cm ⁻³) ^[47] 9,150 (@ 1.902 g cm ⁻³) ^[57]
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		<p>9,540 (@ 1.90 g cm⁻³, $\Delta H_f = 17.9$ kcal/mol, calcd. BKWR, THEOSTAR-T)^[112]</p> <p>9,159 (@ 1.90 g cm⁻³, $\Delta H_f^0 = 613.9$ kJ/kg, calcd., FORTRAN BKW)^[143]</p> <p>9,246 (@ 1.91 g cm⁻³, calcd., Cheetah 7.0)^[171]</p> <p>9,110 (@ 1.89 g cm⁻³)^[183]</p> <p>7,910 (@ 1.60 g cm⁻³)^[183]</p> <p>7,300 (@ 1.40 g cm⁻³)^[183]</p> <p>6,580 (@ 1.20 g cm⁻³)^[183]</p> <p>5,800 (@ 1.00 g cm⁻³)^[183]</p> <p>4,880 (@ 0.75 g cm⁻³)^[183]</p>	<p>9,100 (@ 1.894 g cm⁻³)^[81, 144]</p> <p>6,680 (@ 1.188 g cm⁻³)^[81, 144]</p> <p>6,030 (@ 1 g cm⁻³)^[87]</p> <p>8,110 (@ 1.6 g cm⁻³)^[87]</p> <p>9,110 (@ 1.891 g cm⁻³, cylinder test)^[111]</p> <p>9,150 (@ 1.90 g cm⁻³)^[112]</p> <p>9,124 (@ 1.84 g cm⁻³)^[14]</p> <p>9,100 (@ 1.90 g cm⁻³)^[143]</p> <p>8,410 (@ 1.79 g cm⁻³)^[158]</p> <p>9,120 (@ 1.84 g cm⁻³)^[158]</p> <p>9,090 (@ 1.905 g cm⁻³, $\Delta H_f = 75$ kJ/mol, calcd., JAGUAR)^[163]</p> <p>9,080 (@ 1.89 g cm⁻³, calcd. BKWR)^[183]</p> <p>8,100 (@ 1.60 g cm⁻³, calcd. BKWR)^[183]</p> <p>7,450 (@ 1.40 g cm⁻³, calcd. BKWR)^[183]</p> <p>6,850 (@ 1.20 g cm⁻³, calcd. BKWR)^[183]</p> <p>6,310 (@ 1.00 g cm⁻³, calcd. BKWR)^[183]</p> <p>5,540 (@ 0.75 g cm⁻³, calcd. BKWR)^[183]</p> <p>9,350 (@ 1.89 g cm⁻³, calcd. BKWS)^[183]</p> <p>8,140 (@ 1.60 g cm⁻³, calcd. BKWS)^[183]</p>
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			7,410 (@ 1.40 g cm ⁻³ , calcd. BKWS) ^[183] 6,780 (@ 1.20 g cm ⁻³ , calcd. BKWS) ^[183] 6,200 (@ 1.00 g cm ⁻³ , calcd. BKWS) ^[183] 5,420 (@ 0.75 g cm ⁻³ , calcd. BKWS) ^[183]
V ₀ [L kg ⁻¹]	775		902 ^[15]

Calorimetric heat of detonation, Ornellas method, 25 g cylinder sample, 1.2 cm diameter, detonated in an isothermal calorimetry bomb under a 65 Pa vacuum^[70]:

Material	ρ (g/cm ³)	Heat of detonation [H ₂ O (l) @ 25 °C] (J/g)	Heat of detonation [H ₂ O (l) @ 25 °C] (J/cm ³)	Heat of detonation [H ₂ O (l) @ 25 °C] @ TMD (J/cm ³)
HMX	1.89	6,192	11,703	11,782

Summary of experimental copper cylinder wall velocity data, all samples have a wall thickness/diameter ratio of 0.1, all cylinders were 305 mm long, PETN with $\rho = 1.763$ g/cm³ is the reference explosive^[142]:

Initial ρ , g/cm ³	Inner diameter, mm	Wall thickness, mm	Wall velocity, mm/ μ s at 25.4 mm diameter for $R-R^0$ equal to			Velocity-squared cf. with PETN for the same configuration, % comparison $R-R_0$ equal to		
			6 mm	12.5 mm	19 mm	6 mm	12.5 mm	19 mm
1.894	25.43	2.596	1.650	1.820	1.883	11.9	13.9	10.6
1.188	25.43	2.596	1.173	1.314	1.384	-43.5	-40.6	-40.2

Summary of code calculations with measured detonation velocities and detonation energies derived from JWL's^[142]:

Initial ρ (g/cm ³)	PETN-adjusted BKWR Tiger, LLNL library @ 1,850 K, at v			JCZ3, LLNL library, v			CHEQ V2.4, at v		
	2.2	4.1	6.5	2.2	4.1	6.5	2.2	4.1	6.5
1.894	4	1	2	4	-1	-1	3	-2	-2
1.188	-5	-6	-5	-7	-10	-9	-15	-15	-13

Derivation of the total energy of detonation, E_0 from the measured heat of detonation (the final state is assumed to be at one atmosphere for all gaseous products, including water, at 298 K). Code calculated energies with the 1,800 K freeze are also included^[142]:

Measured ρ (g/cm ³)	Measured confined heat of detonation (kJ/cm ³)	Density from ^[142]	Heat of detonation using density from ^[142]	Energy of detonation, E_0 (kJ/cm ³)			
				From heat of detonation	Freeze at 1,800 K		
					Tiger BKWR	Tiger JCZ3	CHEQ
1.89	−11.70	1.893	−11.71	−11.0	−11.4	−10.9	−11.2
1.20	−6.63	1.188	−6.56	−6.2	−6.5	−6.4	−6.4

Comparison of measured “CJ” temperatures using optical pyrometry^[142]:

Exptl. ρ (g/cm ³)	Maximum measured T (K)	Calculated CJ T (K)			Wavelength (μm)
		Tiger BKWR	Tiger JCZ3	CHEQ	
1.70	2,500–2,800	3,200	4,000	4,200	0.49, 0.69

Desensitized HMX (D-HMX) refers to high-quality β -HMX crystal particles which show less crystal defects and a better morphology than conventional HMX (C-HMX). Values given for D-HMX are for samples with purity of $99.6 \pm 0.1\%$ and mean particle $\rho > 1.9016 \text{ g cm}^{-3}$. Fine grain D-HMX is abbreviated as FD-HMX and large grain D-HMX as LD-HMX^[55]

Critical diameter [cm]	Critical detonation diameter d_{c0} [mm] and specific surface area, S_g [cm ² g ^{−1}] ^[93] :			
	S_g (cm ² g ^{−1})	d_{c0} (mm)	S_g (cm ² g ^{−1})	d_{c0} (mm)
	Monodisperse HMX (fractions)		Polydisperse HMX	
	1,580 (0–90 μm)	1.50	400	2.97
	1,010 (90–160 μm)	2.10	800	1.64
	450 (200–250 μm)	3.10	1,900	0.70
	200 (400–500 μm)	4.80	3,000	0.60
			4,300	0.65
			8,900	0.55

	<p>Critical detonation diameter d_{c0} [mm] and specific surface area, S_g [cm² g⁻¹] @ rel. high density (0.98–0.995)^[93]:</p> <table><tr><td>S_g (cm² g⁻¹)</td><td>d_{c0} (mm)</td><td>S_g (cm² g⁻¹)</td><td>d_{c0} (mm)</td></tr><tr><td>650</td><td>2.15</td><td>2,900</td><td>0.75</td></tr><tr><td>1,500</td><td>1.25</td><td>8,000</td><td>0.45</td></tr></table> <p>d_{c0} (mm) @ mean crystal size (μm)^[93]: 0.40 @ 3, 0.75 @ 10, 1.20 @ 20^[72]</p> <p>d_c in mm, values from ^[16]:</p> <table><tr><td>HMX/wax (%)</td><td>ρ (g/cm³)</td><td>Critical diameters</td></tr><tr><td>90/10</td><td>1.10</td><td>6.0 < d_c < 7.0</td></tr><tr><td>78/22</td><td>1.28</td><td>7.0 < d_c < 8.0</td></tr><tr><td>70/30</td><td>1.42</td><td>8.0 < d_c < 9.0</td></tr></table>	S_g (cm ² g ⁻¹)	d_{c0} (mm)	S_g (cm ² g ⁻¹)	d_{c0} (mm)	650	2.15	2,900	0.75	1,500	1.25	8,000	0.45	HMX/wax (%)	ρ (g/cm ³)	Critical diameters	90/10	1.10	6.0 < d_c < 7.0	78/22	1.28	7.0 < d_c < 8.0	70/30	1.42	8.0 < d_c < 9.0		
S_g (cm ² g ⁻¹)	d_{c0} (mm)	S_g (cm ² g ⁻¹)	d_{c0} (mm)																								
650	2.15	2,900	0.75																								
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HMX/wax (%)	ρ (g/cm ³)	Critical diameters																									
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78/22	1.28	7.0 < d_c < 8.0																									
70/30	1.42	8.0 < d_c < 9.0																									
Critical T [°C]	<p>257 (HMX, isothermal time-to-explosion tests)^[92], 242 (HMX-D₈, isothermal time-to-explosion tests)^[92], 253–255 (exptl. value)^[96, 136], 253 (calcd.)^[96, 136], 913.5 K (est., Joback-Stein method)^[172], 1,234.4 K (Valderrama-Alvarez method)^[172], 927 K^[172], critical T, T_m = 253^[17]</p> <p>Calcd. T_b^[132]:</p> <table><tr><th rowspan="2">Particle size (μm)</th><th rowspan="2">T_i (K)</th><th colspan="2">T_b (K)</th></tr><tr><th>Kissinger</th><th>Ozawa</th></tr><tr><td>350</td><td>551.3</td><td>557.45</td><td>557.31</td></tr><tr><td>160</td><td>546.6</td><td>554.32</td><td>554.11</td></tr><tr><td>90</td><td>544.5</td><td>553.42</td><td>553.13</td></tr><tr><td>50</td><td>539.8</td><td>549.85</td><td>549.48</td></tr><tr><td>40</td><td>538.1</td><td>548.99</td><td>548.56</td></tr></table>	Particle size (μm)	T_i (K)	T_b (K)		Kissinger	Ozawa	350	551.3	557.45	557.31	160	546.6	554.32	554.11	90	544.5	553.42	553.13	50	539.8	549.85	549.48	40	538.1	548.99	548.56
Particle size (μm)	T_i (K)			T_b (K)																							
		Kissinger	Ozawa																								
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160	546.6	554.32	554.11																								
90	544.5	553.42	553.13																								
50	539.8	549.85	549.48																								
40	538.1	548.99	548.56																								
Critical pressure [bar]	52.97 (est., Joback-Stein method) ^[172] , 28.83 (Valderrama-Alvarez method) ^[172]																										
Critical pressure of initiation of explosion [GPa]	Critical pressure of explosion initiation (impact) P_{cr} = 0.65 ± 0.02; σ_{ult} = 135 MPa ^[94] , critical pressure of explosion initiation (DT) P_{cr} = 1.00 ± 0.03 ^[94, 104, 166] , critical pressure of explosion initiation (impact) P_{cr} = 0.65 ± 0.02; σ_{ult} = 130 MPa ^[104] , P_{cr} = 0.99 ± 0.03 (commercial HMX of trade mark “B”, 10–30 μm) ^[121] , P_{cr} = 1.01 ± 0.03 (ultra-fine HMX, ~1.4 μm) ^[121] , P_{cr} = 0.88 ^[126] , σ_{ult} = 155 MPa ^[126]																										
Trauzl test [cm ³ , % TNT]	159–165% TNT ^[16, 26] , 145% TNT ^[14, 27] , 486 cc (expansion in Pb bomb) ^[150] , 428 ^[160] , 480 ^[160]																										

Sand test [g]	60.4 g (200 g bomb) ^[14] , 125% TNT (~96% RDX) ^[16] , 54.4 g–60.4 g sand crushed (cf. 48 g for TNT) ^[27]																								
Ballistic mortar test	150% TNT ^[14, 16, 26, 27]																								
Ballistic pendulum test	170% TNT ^[16]																								
Initiation efficiency	0.30 g LA minimum detonating charge ^[14, 16, 152]																								
Gap test	$\rho = 1.78 \text{ g/cm}^3$, gap test = 11 kbar ^[34] , $G_{50} = 49.5 \text{ mm}$, $\rho = 1.822 \text{ g cm}^{-3}$, rel. $\rho = 95.4\%$ ^[107]																								
LSGT [cm]	<p>$G_{50} = 70.68 \text{ mm}$, $L_{95} = 0.71 \text{ mm}$ (@ 1.07 g cm^{-3})^[17], 61 mm (LANL)^[66], 105 cards^[120]</p> <p>LANL LSGT data from^[16]:</p> <table><tr><td>$\rho \text{ (g/cm}^3\text{)}$</td><td>% voids</td><td>Sensitivity (mm)</td></tr><tr><td>1.07</td><td>43.7</td><td>70.7</td></tr></table> <p>Negative @ 150 cards for a slurry of HMX and butyrolactone-DMSO (72/27) that contained 67% by weight HMX (NOL LSGT)^[148]</p>	$\rho \text{ (g/cm}^3\text{)}$	% voids	Sensitivity (mm)	1.07	43.7	70.7																		
$\rho \text{ (g/cm}^3\text{)}$	% voids	Sensitivity (mm)																							
1.07	43.7	70.7																							
SSGT [cm]	<p>$G_{50} = 8.53 \text{ mm}$, $L_{95} = 0.05 \text{ mm}$ (@ 1.20 g cm^{-3})^[17], $G_{50} = 4.23 \text{ mm}$, $L_{95} = 0.10 \text{ mm}$ (@ 1.79 g cm^{-3})^[17], $G_{50} = 4.04 \text{ mm}$, $L_{95} = 0.13 \text{ mm}$ (@ 1.83 g cm^{-3})^[17], 7.4 mm (NOL)^[66], $P_{90} = 10.81 \text{ kbar}$ (P_{90} = pressure to 90% of TMD, NSWC small-scale gap test)^[84], 2.0 GPa (@ 98% TMD, NSWC)^[167]</p> <p>Data from^[16]:</p> <table><tr><td></td><td>$\rho \text{ (g/cm}^3\text{)}$</td><td>% Voids</td><td>Sensitivity (mm)</td></tr><tr><td rowspan="2">NSWC SSGT</td><td>1.814</td><td>4.7</td><td>8.71</td></tr><tr><td>1.517</td><td>20.3</td><td>11.28</td></tr><tr><td rowspan="4">LANL SSGT</td><td>1.840 (pressed)</td><td>3.2</td><td>3.43</td></tr><tr><td>1.790 (pressed)</td><td>5.8</td><td>4.27</td></tr><tr><td>1.20 (coarse)</td><td>36.8</td><td>8.53</td></tr><tr><td>0.7 (fine crystals)</td><td>63</td><td>6.45</td></tr></table>		$\rho \text{ (g/cm}^3\text{)}$	% Voids	Sensitivity (mm)	NSWC SSGT	1.814	4.7	8.71	1.517	20.3	11.28	LANL SSGT	1.840 (pressed)	3.2	3.43	1.790 (pressed)	5.8	4.27	1.20 (coarse)	36.8	8.53	0.7 (fine crystals)	63	6.45
	$\rho \text{ (g/cm}^3\text{)}$	% Voids	Sensitivity (mm)																						
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	HMX TMD = 1.903 g/cm ³ , data from ^[156] : <table><tr><th rowspan="2">Loading pressure (kpsi)</th><th colspan="2">Density (g/cm³)</th><th rowspan="2">% TMD</th><th colspan="4">Sensitivity (DBG)</th></tr><tr><th>avg.</th><th><i>S</i></th><th>Avg.</th><th><i>g</i></th><th><i>s_m</i></th><th><i>N</i></th></tr><tr><td>8</td><td>1.517</td><td>–</td><td>79.7</td><td>3.526</td><td>0.0172</td><td>0.0216</td><td>20</td></tr><tr><td>16</td><td>1.627</td><td>–</td><td>85.5</td><td>3.475</td><td>0.0548</td><td>0.0328</td><td>20</td></tr><tr><td>32</td><td>1.718</td><td>–</td><td>90.3</td><td>3.508</td><td>0.0102</td><td>0.0097</td><td>20</td></tr><tr><td>64</td><td>1.814</td><td>–</td><td>90.3</td><td>4.644</td><td>0.1546</td><td>0.1023</td><td>20</td></tr></table>	Loading pressure (kpsi)	Density (g/cm ³)		% TMD	Sensitivity (DBG)				avg.	<i>S</i>	Avg.	<i>g</i>	<i>s_m</i>	<i>N</i>	8	1.517	–	79.7	3.526	0.0172	0.0216	20	16	1.627	–	85.5	3.475	0.0548	0.0328	20	32	1.718	–	90.3	3.508	0.0102	0.0097	20	64	1.814	–	90.3	4.644	0.1546	0.1023	20
Loading pressure (kpsi)	Density (g/cm ³)		% TMD	Sensitivity (DBG)																																											
	avg.	<i>S</i>		Avg.	<i>g</i>	<i>s_m</i>	<i>N</i>																																								
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Cook-off <i>T</i> [°C]	210 (confined cook-off <i>T</i>) ^[27] Cook-off tests of standard and modified M47 detonators ^[152] : <table><tr><th rowspan="2">Group designation</th><th colspan="2">Upper charge</th><th colspan="2">Intermediate charge</th><th colspan="2">Base charge</th><th rowspan="2">Cook-off <i>T</i> (°F)</th></tr><tr><th>Explosive</th><th>wt. mg</th><th>Explosive</th><th>wt., mg</th><th>Explosive</th><th>wt. mg</th></tr><tr><td>HMX</td><td>Inert</td><td>10</td><td>Inert</td><td>66</td><td>HMX</td><td>34</td><td>460</td></tr></table>	Group designation	Upper charge		Intermediate charge		Base charge		Cook-off <i>T</i> (°F)	Explosive	wt. mg	Explosive	wt., mg	Explosive	wt. mg	HMX	Inert	10	Inert	66	HMX	34	460																								
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	Explosive	wt. mg	Explosive	wt., mg	Explosive	wt. mg																																									
HMX	Inert	10	Inert	66	HMX	34	460																																								
5 s explosion <i>T</i> [°C]	327 ^[14, 16, 27, 147] , 335 ^[95] , 312.1 ^[118] , 316.0 (thermal aggressed HMX, 40 days @ 85 °C) ^[118] , 318.1 (thermal aggressed HMX, 40 days @ 71 °C) ^[118] , 327 (dec.) ^[152] , 327 (cook-off) ^[152] , 308 (Wood's metal bath, 40 mg) ^[161] 306 ^[14, 16, 27, 152] 380 ^[16, 152] , 380 (no cap used) ^[14, 27] 337 ^[25] , 280 (DTA/TG @ 6 °C/min) ^[34] , 327 ^[139] 327 (USA value) ^[28] , 335 (Russian value) ^[28] 300 ^[74] , 252 (calorimetric measurements) ^[95] Crystal <i>ρ</i> (g cm ⁻³) vs. ignition <i>T</i> (°C) (approx. values) ^[102] : 1.885/237, 1.887/235, 1.8885/241, 1.8885/248, 1.892/252.5, 1.89/256 ^[102] Pin load (N) of friction tests vs. ignition <i>T</i> (°C) ^[102] : 60/237, 80/237, 84/242, 98/248, 130/253, 108/257 ^[102]																																														
10 s explosion <i>T</i> [°C]																																															
0.1 s explosion <i>T</i> [°C]																																															
Explosion <i>T</i> [°C]																																															
5 s ignition <i>T</i> [°C]																																															
Ignition <i>T</i> [°C]																																															
Detonating <i>T</i> [°C]	347 ^[137]																																														
Autoignition <i>T</i> [°C]	234 ^[16]																																														

SBAT (small-scale autoignition test) [°C]	208 (Thiokol) ^[67]										
100 °C heat test [% mass loss]	0.05% mass loss in first 48 h ^[14, 16] , 0.3% mass loss in second 48 h ^[14, 16] , no explosions in 100 h ^[14, 16]										
Thermal stability	No. moles gas per mole HMX produced/no. hours ^[39] : @ 120 °C: 0/22 h, 0/72 ^[39] , @ 220 °C: 4.43/22 h, 4.3/72 ^[39] , @ 320 °C: 4.24/22 h, 5.4/72 ^[39] , 0.04% mass loss @ 120 °C, 48 h (TG) ^[106] , metastable @ RT (α -HMX) ^[150] , stable @ RT (β -HMX) ^[150] , metastable @ RT (γ -HMX) ^[150] , labile @ RT (δ -HMX) ^[150] , 32–39 mm rise in pressure @ 166–167 °C for 5 h (manometric specimen) ^[150]										
LLNL reactivity test	<0.01 cm ³ gas evolved ^[16, 21]										
Vacuum stability test [cm ³ /h]	0.37 cc/40 @ 100 °C ^[14] , 0.45 cc/40 h @ 120 °C ^[14, 152] , 0.62 cc/40 h @ 150 °C ^[14, 16] , 0.1–0.4 mL/g gas evolved after 48 h @ 120 °C ^[17] , 0.07 cm ³ evolved after 48 h @ 120 °C ^[21] , @ 150 °C: 1.2/2 days, 8.9/7 days, 32.9/14 days ^[45] , @ 175 °C: 3.1/2 days, 31.2/7 days ^[45] , @ 100 °C: 0.37 cc gas evolved after 40 h (5 g sample) ^[27] , @ 120 °C: 0.45 cc gas evolved after 40 h (5 g sample) ^[27] , @ 150 °C: 0.62 cc gas evolved after 40 h (5 g sample) ^[27] , 0.06 cm ³ gas produced @ 110 °C for 20 h ^[53, 101, 113] , 0.0 cc/g @ 100 °C/48 h ^[79] , 0.1 cc/g @ 200 °C/h (average for 2 h exposure) ^[79] , mL/5 g/120 °C/48 h: 0.12 LC-HMX ^[55] , 0.24 FC-HMX ^[55] , 0.06 LD-HMX ^[55] , 0.06 FD-HMX ^[55] , 0.4 cm ³ /g (5 g sample, 40 h thermostating @ 120 °C) ^[95] , 0.6 cm ³ /g (5 g sample, 40 h thermostating @ 150 °C) ^[95] , 0.4 mL (5 g sample, 48 h, 120 °C) ^[106] STANAG 4147 test 1B, total gas evolved after 40 h @ 100 °C, values in cc: 0.0699 ^[171]										
Bourdon manometer	0.04 mL•g ⁻¹ @ 120 °C, 48 h ^[106]										
Vapor pressure [mm Hg × 10 ⁷ @ °C]	0.032 @ 97.6 ^[17] , 0.164 @ 108.2 ^[17] , 0.385–0.419 @ 115.6 ^[17] , 2.830–2.870 @ 129.3 ^[17] , 1.51 × 10 ⁻¹¹ Torr @ 66 °C ^[44] , 3.3 × 10 ⁻¹⁴ Torr @ 20 °C ^[52] , 3.33 × 10 ⁻¹⁴ Torr @ 25 °C ^[134] , 3.3 × 10 ⁻¹⁴ mm Hg @ 25 °C ^[141] , 3.00 × 10 ⁻⁹ mm Hg (solid) ^[146] , 3.33 × 10 ⁻¹³ mm Hg (solid) ^[146] , 2.6 ± 0.01 mm Hg @ 20 °C (solid) ^[146] , 5 mm Hg @ 22–25 °C (solid) ^[146] , 3.3 × 10 ⁻¹⁶ mm Hg @ 20 °C (solid) ^[146] , 3.3 × 10 ⁻¹⁴ mm Hg (solid) ^[146] , 5.7 ± 0.1 mm Hg @ 30 °C (solid) ^[146] , 3.01 × 10 ⁻¹⁵ Torr @ 25 °C ^[165, 171] , 3.14 × 10 ⁻¹¹ Torr @ 70 °C ^[165, 171] , 4.37 × 10 ⁻⁹ Torr @ 100 °C ^[165, 171] Vapor pressure of β -HMX ^[30] <table border="1"> <tr> <th>T (K)</th><th>Vapor pressure (Torr)</th></tr> <tr> <td>2,690</td><td>33 × 10⁻⁹</td></tr> <tr> <td>2,615</td><td>18 × 10⁻⁸</td></tr> <tr> <td>2,575</td><td>4 × 10⁻⁸</td></tr> <tr> <td>2,490</td><td>3 × 10⁻⁷</td></tr> </table>	T (K)	Vapor pressure (Torr)	2,690	33 × 10 ⁻⁹	2,615	18 × 10 ⁻⁸	2,575	4 × 10 ⁻⁸	2,490	3 × 10 ⁻⁷
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	$\log_{10} P = 16.855 - 82.96/T \text{ (K) Pa}^{[78]}$ Values from ^[140] : <table><tr><th>$T \text{ (}^\circ\text{C)}$</th><th>Vapor pressure ($\times 10^7 \text{ Torr}$)</th><th>Wt. loss ($\text{g} \times 10^3$)</th><th>Time (s)</th><th>Area (cm^2)</th></tr><tr><td>97.6</td><td>0.0324</td><td>3.7</td><td>3,456,000</td><td>6.33</td></tr><tr><td>108.2</td><td>0.164</td><td>4.6</td><td>860,400</td><td>6.33</td></tr><tr><td>115.6</td><td>0.390</td><td>1.97</td><td>424,080</td><td>2.34</td></tr><tr><td>115.6</td><td>0.385</td><td>1.98</td><td>424,080</td><td>2.38</td></tr><tr><td>115.6</td><td>0.419</td><td>2.09</td><td>424,080</td><td>2.31</td></tr><tr><td>129.3</td><td>2.83</td><td>4.92</td><td>145,800</td><td>2.38</td></tr><tr><td>129.3</td><td>2.87</td><td>4.83</td><td>145,800</td><td>2.31</td></tr></table>	$T \text{ (}^\circ\text{C)}$	Vapor pressure ($\times 10^7 \text{ Torr}$)	Wt. loss ($\text{g} \times 10^3$)	Time (s)	Area (cm^2)	97.6	0.0324	3.7	3,456,000	6.33	108.2	0.164	4.6	860,400	6.33	115.6	0.390	1.97	424,080	2.34	115.6	0.385	1.98	424,080	2.38	115.6	0.419	2.09	424,080	2.31	129.3	2.83	4.92	145,800	2.38	129.3	2.87	4.83	145,800	2.31
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Burn rate [mm/s]	<p>Mass burn rate ($\text{kg/m}^2 \text{ s}$) vs. pressure (MPa) (approx. values)^[91]: 22/0.4, 30/1.1, 40/1.5, 50/2.0, 55/2.9, 70/3.5, 90/4.8, 100/5.5^[91], 3 @ 10 atm. pressure^[109], 15 @ 100 atm. pressure^[109], 100 @ 1,000 atm. pressure^[109], 0.37 (@ 1 atm., SMATCH/FTIR spectroscopy)^[168], 0.5 (@ 1 atm., strand burner)^[168]</p> <p>HMX and HMX-d₈ burn rates (in/s)^[92]:</p> <table><tr><th colspan="2">500 psi (3.55 MPa)</th><th colspan="2">1,000 psi (6.99 MPa)</th><th colspan="2">1,500 psi (10.4 MPa)</th></tr><tr><th>HMX</th><th>HMX-d₈</th><th>HMX</th><th>HMX-d₈</th><th>HMX</th><th>HMX-d₈</th></tr><tr><td>0.257</td><td>0.167</td><td>0.464</td><td>0.306</td><td>0.716</td><td>0.604</td></tr><tr><td>0.253</td><td>0.219</td><td>0.505</td><td>0.311</td><td>0.690</td><td>0.596</td></tr><tr><td>0.284</td><td>0.183</td><td>0.529</td><td>0.320</td><td>0.698</td><td>0.502</td></tr><tr><td>–</td><td>0.192</td><td>–</td><td>0.308</td><td>–</td><td>–</td></tr></table> <p>Burning characteristics of HMX^[108]: $\rho = 1.7 \text{ g cm}^{-3}$, u (linear burning rate) = 0.35 mm/s, m (mass burning rate) = 0.6 kg/m²s, T_s (surface T) = 633 K, Q_s (heat evolved/absorbed in condensed phase) = -0.16 kJ/kg^[108]</p> <p>Burn rate characteristics: pressure interval = 0.3–40.1 MPa, pressure exponent = 0.861, burning rate @ 10 MPa = 18.1 mm/s, strand $\rho = 1.72 \text{ g cm}^{-3}$, adiabatic flame T @ 10 MPa = 3,295 K^[110, 127]</p>	500 psi (3.55 MPa)		1,000 psi (6.99 MPa)		1,500 psi (10.4 MPa)		HMX	HMX-d ₈	HMX	HMX-d ₈	HMX	HMX-d ₈	0.257	0.167	0.464	0.306	0.716	0.604	0.253	0.219	0.505	0.311	0.690	0.596	0.284	0.183	0.529	0.320	0.698	0.502	–	0.192	–	0.308	–	–				
500 psi (3.55 MPa)		1,000 psi (6.99 MPa)		1,500 psi (10.4 MPa)																																					
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HMX combustion parameters, subatmospheric, atmospheric and high pressure @ $T_0 = 20\text{ }^{\circ}\text{C}^{[116]}$:

p (MPa)	0.05	0.075	0.1	20	30	50
m (g/cm ² c)	0.05	0.06	0.07	3.4	4.4	5.8
T_s (°C)	307	309	312	551	565	581
$(dT/dx)_0 \cdot 10^{-4}$ (K/cm)	9.5	9	8	42.5	42.7	47.8
q (cal/g)	228	180	138	20	16	14
q_r (cal/g)	3	4	7	6	5	4
Q (cal/g)	−92	−44	−4.5	170	220	230
l (mkm)	345	286	268	–	–	–
l_m (mkm)	51	47	50	–	–	–
$ks \cdot 10^{-4}$ (cal/cm•K•s)	5	5	6	28	30	40
T_f (°C)	1,600	1,800	2,100	2,750	2,780	2,800
L (mm)	0.6	1.2	1.0	0.3	0.22	0.18
l_R (mkm)	13	13	14	1.85	1.54	1.56
d (mkm)	87	73	64	1.6	1.2	1.0
L/d	7	16	16	190	180	180
W	0	0.14	0.26	0.92	0.95	0.98
F_s (kcal/cm ³ s)	−2.3	−2.3	−1.0	4,060	6,590	8,990
F_0 (kcal/cm ³ s)	1.2	1.5	1.7	450	600	1,250

HMX combustion parameters^[116]:

p (MPa)	0.5			1			2			5			10		
	-170	20	100	-170	20	100	-170	20	100	-170	20	100	-170	20	100
T_0 (°C)															
m (g/cm ² ·s)	0.19	0.26	0.36	0.34	0.46	0.58	0.6	0.78	0.94	1.22	1.42	1.68	2.04	2.2	2.5
T_s (°C)	367	385	404	403	424	439	441	461	474	496	505	514	523	527	533
$(dT/dx)_0 \cdot 10^{-4}$ (K/cm)	21.3	12.7	14.8	25.2	18.5	18.6	26.7	23	24.3	26.5	28	33.3	31.5	36	38.7
q (cal/g)	146	65	56	100	54	46	63	43	38	33	30	30	24	26	25
q_f (cal/g)	16	12	8	16	12	9	15	12	10	13	11	10	10	9	8
Q (cal/g)	56	94	82	114	120	105	166	146	125	218	176	150	240	192	165
l (mkm)	100	75	60	55	45	42	40	38	32	26	24	22	20	18	17
l_m (mkm)	12	20	32	18	25	34	15	20	25	12	17	19	10	14	18
$ks \cdot 10^{-4}$ (cal/cm·K·s)	5.6	5.8	6.3	5.6	6.0	7.0	6.6	8.7	9.2	9.7	10	11	12	12	13
T_f (°C)	2,450	2,450	2,450	2,450	2,500	2,500	2,600	2,700	2,750	2,600	2,750	2,850	2,600	2,750	2,850
L (mm)	0.65	0.7	0.7	0.8	0.8	0.8	0.5	0.5	0.6	0.4	0.45	0.5	0.3	0.34	0.25
l_R (mkm)	14	6.2	6.0	3.4	4.0	4.5	2.8	3.7	3.9	1.3	1.5	1.6	1.6	1.2	1.3
d (mkm)	48	35	25	26	19	15	16	12	10	8	7	6	5	4.8	4.2
L/d	14	20	28	30	42	53	30	42	60	50	64	80	60	70	60
W	0.42	0.57	0.57	0.58	0.64	0.65	0.73	0.72	0.72	0.88	0.82	0.80	0.94	0.87	0.85
F_s (kcal/cm ³ ·s)	25.8	44.0	58.0	126	150	154	390	340	343	2,095	1,800	1,700	1,900	3,760	3,380
F_0 (kcal/cm ³ ·s)	—	10	—	—	30	—	—	55	—	—	270	—	—	350	—

Pressure and temperature sensitivities of HMX burning rate @ 20 °C^[116]:

p (MPa)	0.5	1	2	5	10
n	0.82	0.78	0.72	0.64	0.58
$b \cdot 10^2, 1/K$	0.26	0.24	0.18	0.14	0.15

Burning rates of pressed HMX @ various pressures (atm.), paper tube method (approx. values taken from graphs)^[151]:

HMX powder characteristics (particle diameter/mean loading ρ)	apparent mass burning rate ($\text{g cm}^{-2} \text{ s}^{-1}$)/@ pressure (atm.)
200–600 μ /1.20 g cm^{-3}	10/25, 20/23, 25/25, 30/27, 40/35
104–124 μ /1.05 g cm^{-3}	3/25, 20/45, 40/65
64–76 μ /1.07 g cm^{-3}	2/40, 4/50, 15/70, 34/100
53–64 μ /1.08 g cm^{-3}	3/90, 18/110, 25/120, 45/150
approx. 5 μ /1.02 g cm^{-3}	2/25, 3/50, 4/155, 6/200

Results of burning rates in unconstricted (a), (b) and constricted (c) tubes using coarse HMX (200–600 μ particle diameter), Fig. 15^[151]:

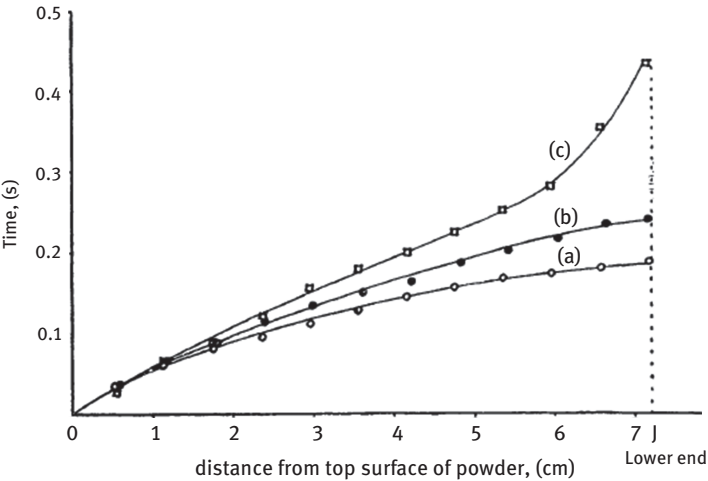
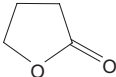
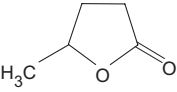
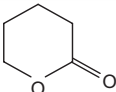
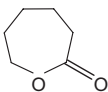


Fig. 15: Typical distance against time plots of the flame front for HMX; nitrogen pressure 27.2 atm; particle diameter approximately 200–600 μ ; loading density 1.08 g/cm^3 ^[151].

	Dependence of burning rate of volatile explosives on pressure ^[155] :					
	$\delta = \rho/\rho_{\max}$	Coefficients in formulae, $m(\text{gm cm}^{-2} \text{ s}^{-1})$ $= 1 + b p_{\text{atm}}^v$			Pressure, atm.	
		a	b	N		
	0.875	–	0.0436	0.90	12–205	
	Values of the mass burning rate of HMX for two values of δ at different pressures ^[155] :					
	Pressure, atm.	$m, \text{gm cm}^{-2} \text{ s}^{-1}$		Pressure, atm.	$m, \text{gm cm}^{-2} \text{ s}^{-1}$	
		$\delta = 0.54$	$\delta = 0.87$		$\delta = 0.54$	$\delta = 0.87$
	12.6	0.48	0.49	154	3.31	3.91
	27.2	0.88	–	205	5.13	5.20
	52	1.43	1.48			
Particle size	Particle size of fine (F) and large grain (L) conventional (C-HMX) and desensitized HMX (D-HMX), particle sizes measured using laser particle sizer ^[55] :					
	Sample	Mean particle size (μm)	Median particle size (μm)	D_{10} (μm)	D_{90} (μm)	
	LD-HMX	153.4	153.3	81.4	224.9	
	LC-HMX*	162.4	185.3	88.8	227.6	
	FD-HMX	15.5	16.3	8.4	24.7	
	FC-HMX	26.9	18.0	4.2	62.1	
*LC-HMX refers to conventional HMX which has been sieved						
25–180 μm (average particle size = 94.1 μm) HMX obtained via solvent/nonsolvent (DMSO/ H_2O) recrystallization process ^[65]						
Solubility [g/mL]	5.0 mg/L H_2O @ 20 °C ^[52, 146] , 4.80 mg/L H_2O @ 25 °C ^[58] , aqueous solubility = 5 mg/L @ 25 °C ^[134, 146] , 0.0045 g/L in H_2O @ 25 °C ^[138] , 4.5 mg/L in H_2O @ 25 °C ^[141] , insoluble in water ^[16] , 0.003 g/100 mL CHCl_3 ^[16] , 0.002 g/100 mL CCl_4 ^[16] , 0.144 g/100 mL dioxane ^[16] , insoluble in CS_2 ^[16] , 6.6 mg/L @ 20 °C ^[146] , 150 mg/L ^[146] , 6.60 mg/L ^[146] , 6.63 mg/L ^[146] , 2.6 mg/L ^[146] , 5 mg/L ^[146] , 5.0×10^{-3} mg/mL in H_2O @ 25 °C ^[165]					

Solubility in less common organic solvents^[76]:

Solvent	Structure	Solubility (g) of HMX in 100 g solvent	
		@ 23 °C	@ 120 °C
γ-Butyrolactone		11.0	48.1
γ-Valerolactone		9.2	35.5
δ-Valerolactone		6.5	35.7
ε-Caprolactone		6.8	38.3

Recryst. from acetone, cyclohexane or γ-butyrolactone produces β-HMX crystals^[76]

Mass fraction of HMX in acetone/2-propanol mixtures ($m(\text{HMX})/m(\text{solvent})$) vs. mole fraction of 2-propanol ($n(2\text{-propanol})/n(\text{total solvent})$) (approx. values)^[88]: 0.029 mass fraction/0 mole fraction, 0.020/0.1, 0.014/0.2, 0.009/0.3, 0.006/0.4, 0.003/0.5, 0.002/0.6, 0.001/0.7, 0.0005/0.8, 0.00/0.9, 0.00/1^[88]

Mass fraction of HMX in acetonitrile/2-propanol mixtures ($m(\text{HMX})/m(\text{solvent})$) vs. mole fraction of 2-propanol ($n(2\text{-propanol})/n(\text{total solvent})$) (approx. values)^[88]: 0.021 mass fraction/0 mole fraction, 0.015/0.1, 0.009/0.2, 0.007/0.3, 0.005/0.4, 0.003/0.5, 0.002/0.6, 0.001/0.7, 0.0005/0.8, 0.00/0.9, 0.00/1^[88]

Solubility (g HMX/g solv.) @ different temperatures^[115]:

Temperature (°C)	Solvent	
	Butyrolactone	Propylene carbonate
20	0.13	0.02
40	0.17	0.055
60	0.21	0.09
80	0.275	0.13

Solubility of HMX in different solvents @ different T (g (HMX)/g (solvent))^[125]: 0.125 (butyrolactone @ 20 °C)^[125], 0.025 (PC @ 20 °C)^[125], 0.024 (cyclohexanone @ 20 °C)^[125], 0.18 (butyrolactone @ 40 °C)^[125], 0.05 (PC @ 40 °C)^[125], 0.04 (cyclohexanone @ 40 °C)^[125], 0.225 (butyrolactone @ 60 °C)^[125], 0.075 (PC @ 60 °C)^[125], 0.05 (cyclohexanone @ 60 °C)^[125], 0.275 (butyrolactone @ 80 °C)^[125], 0.075 (PC @ 80 °C)^[125], 0.06 (cyclohexanone @ 80 °C)^[125], practically insoluble in H₂O^[137], similar solubility in other solvents with that of RDX^[137], practically insoluble in water^[139], soluble in other solvents which dissolve RDX^[139]

Data from^[16]:

Solvent	g HMX dissolved per 100 g soln.	T (°C)
DMF	4.4	25
Nitrobenzene	0.129	25
1,2-Dichloroethane	0.125	70
Acetic acid	0.0375	25
Acetone	0.96	25
Acetonitrile	1.98	25
Cyclohexanone	2.11	25
Ethylacetate	0.02	25
Ethylbromide	0.02	25
Methy ethyl ketone	0.46	25
Nitroethane	0.172	25
Nitromethane	0.778	25
Triethylphosphate	1.75	25

Solubility of HMX by volume^[16]:

Solvent	g HMX dissolved per 100 mL of soln.
γ -butyrolactone	21.0
Cyclopentanone	1.3
Cylohexanone	5.2
Acetone	2.2
Acetonitrile	2.0
Nitromethane	1.1
Nitroethane	0.03
Methylisobutylketone	1.8

Solubility of HMX (g/100 g of solvent) after 5 mins. stirring^[148]:

Solvent	25 °C	60 °C	80 °C	98 °C
DMSO	57	68		89
DMF	Solvate			
<i>N</i> -Methylpyrrolidone	Solvate			
Dimethylacetamide	Solvate			
Butyrolactone	12	20		35
Acetone	2.8	4.2		
Acetonitrile	2.0		7.3	
Cyclohexanone	1.0			8.9
Hexamethylphosphoramide	1.4			37

Solubilities of HMX in binary solvent mixtures @ 25 °C (g/100 g solvent) after 5 mins. stirring^[148]:

Solvent	HMX
DMSO	57
NMP	Solvate
NMP 79.20% DMSO 20.8%	Solvate
DMF	Solvate
DMF 71.7% DMSO 28.3%	Solvate
Butyrolactone	12
Butyrolactone 73.0% DMSO 27.0%	26

Solubility of HMS in butyrolactone-DMSO (72/27) (g/100 g solvent) after 5 mins. stirring^[148]:

T	0°C	25 °C	60 °C	98 °C
Solubility	20	26	33	49

Comparison of solubilities (g/100 g solvent) after 5 mins. and 30 mins. stirring @ 25 °C^[148]:

Sample	Solvent	5 min stirring	30 min stirring
HMX	DMSO	57	58
HMX	Butyrolactone	12	13

Insoluble in MeOH, EtOH, benzene, toluene, xylene and Et₂O^[150], poorly soluble in dichloroethane, aniline, nitrobenzene and dioxane^[150], 0.003% solubility in water @ 15–20 °C^[150], 0.02% solubility in water @ 100 °C^[150]

Data from^[150]:

T (°C)	Solubility of HMX, %			
	Acetone	Butylacetate	Aniline	Mononitrotoluene
22	2.10	1.14	–	–
27	2.65	–	0.35	–
37	3.52	–	–	–
44	4.0	3.38	–	0.89
56	4.13	–	0.49	1.23
60	–	0.57	–	–
68	–	–	0.67	–
78	–	–	0.89	–
83	–	–	1.05	–
90	–	–	1.19	–
99	–	–	1.38	–
104	–	0.77	1.61	1.60
122	–	0.88	2.09	1.98

4.46×10^{-3} g/L in H₂O^[172], 2.7×10^{-3} g/L in H₂O @ 298.15 K (est., Klopman method)^[172], 2.16×10^{-3} g/L in H₂O (@ 298.15 K, est., COSMOtherm method)^[172]

	<p>Data from^[17]:</p> <table><tr><th rowspan="2">Solvent</th><th colspan="3">g dissolved/100 g solvent</th></tr><tr><th>20 °C</th><th>40 °C</th><th>60 °C</th></tr><tr><td>Glacial acetic acid</td><td>0.037</td><td>0.044</td><td>0.090</td></tr><tr><td>70% acetic acid</td><td>–</td><td>0.033</td><td>0.103</td></tr><tr><td>Acetic anhydride</td><td>–</td><td>1.29</td><td>1.94</td></tr><tr><td>Anhydrous acetone</td><td>2.4</td><td>3.4</td><td>–</td></tr><tr><td>70% acetone</td><td>0.66</td><td>1.20</td><td>–</td></tr><tr><td>Acetonitrile</td><td>–</td><td>3.07</td><td>4.34</td></tr><tr><td>Cyclohexanone</td><td>–</td><td>5.91</td><td>7.17</td></tr><tr><td>DMF</td><td>–</td><td>6.1</td><td>11.1</td></tr><tr><td>DMSO</td><td>–</td><td>45.5</td><td>47.2</td></tr></table>	Solvent	g dissolved/100 g solvent			20 °C	40 °C	60 °C	Glacial acetic acid	0.037	0.044	0.090	70% acetic acid	–	0.033	0.103	Acetic anhydride	–	1.29	1.94	Anhydrous acetone	2.4	3.4	–	70% acetone	0.66	1.20	–	Acetonitrile	–	3.07	4.34	Cyclohexanone	–	5.91	7.17	DMF	–	6.1	11.1	DMSO	–	45.5	47.2
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Batch sorption	$K_{ow} = 1.46 \pm 0.001^{[58]}$, K_d (sandy soil) = 0.07 ± 0.11 L/kg ^[58] , K_d (clayed soil, organic rich) = 5.78 ± 0.33 L/kg ^[58]																																											
Log K_{ow}	0.26 ^[134, 165] , 0.06 ^[134] , 0.17 @ 25 °C ^[138, 141] , $K_{ow} = 1.15$ L/kg ^[146] , $K_{ow} = 3.9$ L/kg ^[146] , $K_{ow} = 2.6$ L/kg ^[146] , $K_{ow} = 0.6$ L/kg ^[146] , $K_{ow} = 0.13$, 0.06 L/kg ^[146] , $K_{ow} = 0.061$ L/kg ^[146] , $K_{ow} = 5.9$ L/kg ^[146] , $K_{ow} = 1.82^{[165]}$, 0.165 (@ 21 °C, measured) ^[172] , 1.13 (@ 298.15 K, est., Broto method) ^[172] , 1.39 (@ 298.15 K, est., Ghose method) ^[172] , 0.42 (@ 298.15 K, est., COSMOtherm method) ^[172]																																											
Log K_{oc}	0.54 ^[134, 165] , $K_{oc} = 3.47$ L/kg ^[146] , $K_{oc} = 5.4$ L/kg ^[146] , $K_{oc} = 2.83$ L/kg ^[146] , $K_{oc} = 6.310$ L/kg ^[146] , $K_{oc} = 2.8$ L/kg ^[146] , $K_{oc} = 3.46^{[165]}$																																											
Hygroscopicity	0.0% @ 30 °C, 95% RH ^[14] , nonhygroscopic @ 30% and 95% RH ^[16, 147] , non-hygroscopic ^[139]																																											
Photosensitivity	<p>Properties of aqueous HMX solns. before and after UV irradiation in continuous flow system determined by LC and TLC^[62]:</p> <table><tr><th>UV exposure time (h)</th><th>LC (HMX, ppm)</th><th>pH</th><th>TLC detectable products</th></tr><tr><td>0</td><td>5.6</td><td>6.9</td><td>HMX</td></tr><tr><td>2</td><td>0</td><td>3.6</td><td>0</td></tr><tr><td>4</td><td>0</td><td>3.2</td><td>0</td></tr><tr><td>6</td><td>0</td><td>3.1</td><td>0</td></tr><tr><td>24</td><td>0</td><td>3.0</td><td>0</td></tr></table>	UV exposure time (h)	LC (HMX, ppm)	pH	TLC detectable products	0	5.6	6.9	HMX	2	0	3.6	0	4	0	3.2	0	6	0	3.1	0	24	0	3.0	0																			
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	<p>UV, 0.1% H₂O₂ static treatment of aqueous HMX solutions^[62]:</p> <table><tr><th>UV exposure time (h)</th><th>ppm H₂O₂</th><th>TOC analyzer</th></tr><tr><td>0</td><td>1,000</td><td>—*</td></tr><tr><td>0.5</td><td>~ 100</td><td>—</td></tr><tr><td>1</td><td>> 12, > 50</td><td>—</td></tr><tr><td>5</td><td>0</td><td>—</td></tr></table> <p>*sensitivity of TOC analyzer insufficient to determine concentration</p> <p>HMX is readily degraded photochemically^[134], aqueous HMX solns. photolyzed by sunlight within days^[134], unaffected by light^[150]</p>	UV exposure time (h)	ppm H ₂ O ₂	TOC analyzer	0	1,000	—*	0.5	~ 100	—	1	> 12, > 50	—	5	0	—	
UV exposure time (h)	ppm H ₂ O ₂	TOC analyzer															
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5	0	—															
Compatibility	<p>CL-20 does not influence the dec. of HMX @ ambient pressure^[93], the dec. of CL-20 is accelerated by HMX @ higher pressure and the acceleration effect is almost independent of HMX content^[93], vacuum test of HMX/TNAZ (60/40) mixtures, 110 °C, 20 h, $\rho = 1.85 \text{ g cm}^{-3}$, (98.7% TMD), vol. of gas = $0.04 \text{ cm}^3/\text{g}$^[101], very dil. sulfuric and nitric acids do not decompose HMX on boiling for 6 h^[150]</p> <p>VTS compatibility (STANAG 4147 test 1B, 2.5 g of compound 1 mixed with 2.5 g of compound 2, total gas evolved after 40 h @ 100 °C, values in cc)^[171]: 0.2323 (TNBA), (DNMT), 1.3033 (PiPE), (DNP), (DNGU), 0.3372 (LLM-105), 0.226 (HK-56), concluding that all are compatible with HMX^[171]</p>																
Heat capacity [cal/(g K)]	<p>$C_p = 0.2080 + 2.761 \times 10^{-3} T \text{ (K) (J/g/K)}$^[78]</p> <p>$C_p^{298} \text{ (cal mol}^{-1} \text{ K}^{-1})$: 75.1 ($\alpha$-)^[162], 73.6 ($\beta$-)^[162], 75.6 ($\gamma$-)^[162], 89.5 ($\delta$-)^[162]</p> <p>$\beta$-HMX, initial $\rho = 1.85 \text{ g cm}^{-3}$^[71]:</p> <table><tr><th>T (K)</th><th>Heat capacity (cal/(g K))</th></tr><tr><td>298</td><td>0.24</td></tr><tr><td>373</td><td>0.30</td></tr><tr><td>433</td><td>0.34</td></tr><tr><td>563</td><td>0.40</td></tr><tr><td>623</td><td>0.46</td></tr><tr><td>773</td><td>0.55</td></tr><tr><td>>1,273</td><td>0.55</td></tr></table>	T (K)	Heat capacity (cal/(g K))	298	0.24	373	0.30	433	0.34	563	0.40	623	0.46	773	0.55	>1,273	0.55
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Specific heat [cal/g/°C]	recryst. HMX ^[14, 16] :																											
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Thermal conductivity [cal/(cm g K)]	β -HMX and δ -HMX, initial $\rho = 1.85 \text{ g cm}^{-3}$ [71]:																											
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	$7 \times 10^{-4} \text{ cal/cm s }^\circ\text{C}$ ^[167] , $1.2 \times 10^{-3} \text{ cal/s cm }^\circ\text{C}$ @ 25°C ^[17] , $9.7 \times 10^{-4} \text{ cal/s cm }^\circ\text{C}$ @ 160°C ^[17]																											

Enthalpy for phase changes [kJ mol ⁻¹]	$\beta\text{-HMX} \rightarrow \delta\text{-HMX}, \Delta H^\circ = 9.8 \pm 0.1$ (exptl. value) ^[73] , $\beta\text{-HMX} \rightarrow \delta\text{-HMX}, \Delta H^\circ = 9.832$ (Hall's value) ^[73] , $\delta\text{-HMX} \rightarrow \text{liq. HMX}, \Delta H^\circ = 69.9 \pm 4.2$ (exptl. value) ^[73] , $\beta\text{-HMX} \rightarrow \delta\text{-HMX}$, enthalpy of phase change = 30 J/g ^[129] , $\Delta H_{\text{phase transition}} = 1.77 \pm 0.05$ kcal/mol ($\alpha \rightarrow \delta$) ^[162] , $\Delta H_{\text{phase transition}} = 2.34 \pm 0.03$ kcal/mol ($\beta \rightarrow \delta$) ^[162] , $\Delta H_{\text{phase transition}} = 0.67 \pm 0.02$ kcal/mol ($\gamma \rightarrow \delta$) ^[162] , $\Delta H_{\text{phase transition}} = 1.67 \pm 0.03$ kcal/mol ($\beta \rightarrow \gamma$) ^[162] , $\Delta H_{\text{phase transition}} = 1.10 \pm 0.05$ kcal/mol ($\alpha \rightarrow \gamma$) ^[162] , $\Delta H_{\text{phase transition}} = 0.57 \pm 0.05$ kcal/mol ($\alpha \rightarrow \beta$) ^[162]																																																
Enthalpy change for sublimation, ΔH_{sub} [kJ mol ⁻¹]	185.762 ± 1.5 (β -HMX, calcd.) ^[73] , 174.930 ± 1.5 (δ -HMX, calcd.) ^[73]																																																
Heat of sublimation	41.89 kcal (molar heat of sublimation, β -HMX) ^[140] , 141.4 cal/g (specific heat of sublimation, β -HMX) ^[140] , 41.9 kcal/mol (β -HMX) ^[174] , 39.3 kcal/mol (α -HMX) ^[174] , 38.0 kcal/mol (γ -HMX) ^[174] ,																																																
Enthalpy change for vaporization, ΔH_v [kJ mol ⁻¹]	105.067 ± 4.2 (liq. HMX) ^[73] , 174.5 ^[165] , 174.7 (est.) ^[171]																																																
Exploding foil shock detonation	HMX flyer plate velocity = 2.37 mm/μs ^[92] , HMX-d ₈ flyer plate velocity = 2.27 mm/μs ^[92]																																																
Acceleration ability	<div>Calculated and measured cylinder velocities; R–R_0 (mm) (R = current value of outer cylinder radius, R_0 = initial outer radius of cylinder, Cu cylinder)^[97]:</div> <table><tr><th></th><th>δ (g cm⁻³)</th><th colspan="6">R–R_0 (mm)</th></tr><tr><th></th><th></th><th>4</th><th>5</th><th>7</th><th>10</th><th>12</th><th>15</th></tr><tr><td>Exptl.</td><td>1.81</td><td>1.59</td><td>1.65</td><td>1.72</td><td>1.77</td><td>1.80</td><td>1.83</td></tr><tr><td>Calcd.</td><td>1.81</td><td>1.59</td><td>1.65</td><td>1.72</td><td>1.77</td><td>1.80</td><td>1.83</td></tr><tr><td>Exptl.</td><td>1.73</td><td>1.53</td><td>1.59</td><td>1.66</td><td>1.71</td><td>1.74</td><td>1.77</td></tr><tr><td>Calcd.</td><td>1.73</td><td>1.53</td><td>1.59</td><td>1.66</td><td>1.71</td><td>1.74</td><td>1.77</td></tr></table>		δ (g cm ⁻³)	R – R_0 (mm)								4	5	7	10	12	15	Exptl.	1.81	1.59	1.65	1.72	1.77	1.80	1.83	Calcd.	1.81	1.59	1.65	1.72	1.77	1.80	1.83	Exptl.	1.73	1.53	1.59	1.66	1.71	1.74	1.77	Calcd.	1.73	1.53	1.59	1.66	1.71	1.74	1.77
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Particle size	Particle size and particle size distribution (span = $(X_{84.3}-X_{16.3})/2\bullet X_{50.3}$), measured by laser light scattering ^[98] :																														
	<table><tr><td>Sample</td><td>$X_{50.3}$</td><td>Span</td><td>Sample</td><td>$X_{50.3}$</td><td>Span</td></tr><tr><td>Type B, class 1 (Dyno Nobel, Norway)</td><td>161.6</td><td>0.640</td><td>Class 1, NSO 112 (Eurengo)</td><td>385.7</td><td>0.629</td></tr><tr><td>Type B, 10–15 m (Dyno Nobel, Norway)</td><td>15.5</td><td>0.411</td><td>Class 5, NSO 155 (Eurengo)</td><td>39.8</td><td>0.409</td></tr><tr><td>RS-HMX, class 1 (Dyno Nobel, Norway)</td><td>375.6</td><td>0.432</td><td>Recryst. in PC (Fraunhofer ICT)</td><td>103.9</td><td>0.927</td></tr><tr><td>RS-HMX, class 5 (Dyno Nobel, Norway)</td><td>7.1</td><td>0.586</td><td>Recryst. in γ-BI (Fraunhofer ICT)</td><td>285.9</td><td>0.832</td></tr></table>	Sample	$X_{50.3}$	Span	Sample	$X_{50.3}$	Span	Type B, class 1 (Dyno Nobel, Norway)	161.6	0.640	Class 1, NSO 112 (Eurengo)	385.7	0.629	Type B, 10–15 m (Dyno Nobel, Norway)	15.5	0.411	Class 5, NSO 155 (Eurengo)	39.8	0.409	RS-HMX, class 1 (Dyno Nobel, Norway)	375.6	0.432	Recryst. in PC (Fraunhofer ICT)	103.9	0.927	RS-HMX, class 5 (Dyno Nobel, Norway)	7.1	0.586	Recryst. in γ -BI (Fraunhofer ICT)	285.9	0.832
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	PC = propylene carbonate, γ -BI = γ -Butyrolactone																														
	Effect of bead milling (time (h)) on crystal size (nm) ^[99] : 0/452.9 ^[99] , 1.0/176.2 ^[99] , 5.9/171.1 ^[99]																														
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HMX, recryst. from butyrolactone (0.02% RDX impurity)	285.9	0.832																													
Cylinder test results	<p>ρ = 1,891 kg/m³, VoD = 9,110 m/s, $P_{\text{C-J}}$ = 42.0 GPa, EG = 4,669 kJ/kg (calcd. based on VoD, $P_{\text{C-J}}$ results), v_{G} = 3,056 m/s, det. energy (lit. value), E_0 = 10.5 GPa, E_{ocal} (calcd. from cylinder test data = 11.09 GPa)^[111]</p> <p>Data from^[17]:</p> <table><tr><td rowspan="2">Density (g/cm³)</td><td colspan="2">Cylinder wall velocity (mm/μs) at</td></tr><tr><td>$R-R_0$ = 5 mm</td><td>$R-R_0$ = 19 mm</td></tr><tr><td>1.891</td><td>1.65</td><td>1.86</td></tr></table>	Density (g/cm ³)	Cylinder wall velocity (mm/ μ s) at		$R-R_0$ = 5 mm	$R-R_0$ = 19 mm	1.891	1.65	1.86																						
Density (g/cm ³)	Cylinder wall velocity (mm/ μ s) at																														
	$R-R_0$ = 5 mm	$R-R_0$ = 19 mm																													
1.891	1.65	1.86																													
Heat of soln. [kcal/mol]	Nitromethane: 4.4 (β -HMX) ^[129] , 1.5 (δ -HMX) ^[129] , 4.4 (β -HMX, Holston Defense Corp.) ^[174] , 3.8 (α -HMX, Holston Defense Corp.) ^[174] , 3.7 (δ -HMX, Holston Defense Corp.) ^[174] , 1.5 (γ -HMX, Holston Defense Corp.) ^[174]																														

Thermal expansion	Anisotropic volumetric thermal expansion = 0.0131%/K on heating β -HMX ^[129]																
Energy of melting [kJ/mol]	DSC @ 5 °C/min, 0.5–2.5 mg sample, Al pan with perforated cover, N ₂ ^[132] : 419.71 (350 μ m particle size, Kissinger's method) ^[132] , 373.06 (160 μ m particle size, Kissinger's method) ^[132] , 330.72 (125 μ m particle size, Kissinger's method) ^[132] , 285.49 (90 μ m particle size, Kissinger's method) ^[132] , 250.17 (50 μ m particle size, Kissinger's method) ^[132] , 229.9 (40 μ m particle size, Kissinger's method) ^[132] , 429.29 (350 μ m particle size, Ozawa's method) ^[132] , 382.34 (160 μ m particle size, Ozawa's method) ^[132] , 339.96 (125 μ m particle size, Ozawa's method) ^[132] , 294.69 (90 μ m particle size, Ozawa's method) ^[132] , 259.33 (50 μ m particle size, Ozawa's method) ^[132] , 239.01 (40 μ m particle size, Ozawa's method) ^[132] , $\Delta H_m = 45.0$ ^[172]																
Diffusion coefficient [cm ² /s]	0.063 (air) ^[134, 146] , 0.78 (air) ^[146] , 6.02×10^{-6} (water) ^[134, 146]																
Biodegradation	Aerobic biotransformation has little effect on the presence of HMX in the environment ^[134] , certain anaerobic sludge treatments with elevated nutrient levels result in effective transformation ^[134] , biodegradability soil (aerobic) = negligible ^[146] , biodegradability soil (anaerobic) = accelerated ^[146]																
Half life in soil [days]	14,235 ^[146] , 1.17×10^6 ^[146]																
Half-life in water [days]	0.46–0.5 ^[146] , 17.7 ^[146] , 1.4 ^[146]																
Hardness	2.3 (Moh's scale) ^[14, 16] , 41.3 ± 1 kg mm ⁻² (single crystals, ~5 mm diameter, @ 20 °C, Vicker's hardness) ^[145]																
Laser ignition	Detonated by Q-switched laser, 6,943 Å when HMX is under 13,500 lb/in ² ^[16] successful detonation, if HMX sample compressed against glass plate (Ruby laser (6,943 Å) both in free running and Q-switch modes) ^[152]																
Heat of decomposition [cal/g]	<div>855 (est.)^[149]</div> <div>Thermal dec. temperature and exothermic quantity for three types of HMX samples^[169]:</div> <table><tr><td>Sample</td><td>t_i (°C)</td><td>T_p (°C)</td><td>Q (J/g)</td></tr><tr><td>α-HMX</td><td>281.1</td><td>334.6</td><td>1,063</td></tr><tr><td>HMX-I</td><td>281.6</td><td>335.1</td><td>1,035</td></tr><tr><td>β-HMX</td><td>282.1</td><td>335.6</td><td>1,014</td></tr></table>	Sample	t_i (°C)	T_p (°C)	Q (J/g)	α -HMX	281.1	334.6	1,063	HMX-I	281.6	335.1	1,035	β -HMX	282.1	335.6	1,014
Sample	t_i (°C)	T_p (°C)	Q (J/g)														
α -HMX	281.1	334.6	1,063														
HMX-I	281.6	335.1	1,035														
β -HMX	282.1	335.6	1,014														
Kast brisance	4.2 mm (@ 1.53 g cm ⁻³) ^[150]																
Flash point [°C]	291 ^[150]																

Reflectance tests	Reflectance tests @ 10,600 Å (continuous wave yttrium garnet aluminum laser, pressed explosive) ^[154] :					
	Material	Particle size, mesh	Loading pressure, 10 ³ psi		Reflectance, %	
	HMX	Through 325	10		80.0	
BIC test	<dp/dt≥203 psi/μs, <E≥163 J/g ^[157]					
CRT	≤0.1 cm ³ /g (22 h @ 120 °C under 1 atm. He) ^[159]					
Small-scale shock reactivity test	Used sample weight = 534 mg, dent = 972 mg SiO ₂ ^[181]					
Radiation sensitivity	Effect of 60 MeV electron irradiation on explosives, samples tested at 100 cm with NOL apparatus ^[189] :					
	Weight (mg)	Dose (R)	Dose rate (R/s)	Weight loss	Color change	Test Results
	7.7	1.14 × 10 ⁹	1.7 × 10 ⁶			Impact No explosion
	Critical doses and T to initiate HMX by pulsed high-energy electrons, ^a = estimated 50% initiation dose ^[189] :					
	Explosive	Critical dose (J/g)		Ignition T (°C)		
		Calcd.	Exptl. ^a	Calcd.	Exptl.	
	HMX	156.1 > 167	310	335		
	Data from ^[185] :					
	Exposure rate (R/h)	Total dose (R)	Vacuum stability test			
			200 °C (cc/2 g/2 h)			
		Control	0.42			
	8 × 10 ⁵	1.3 × 10 ⁷	1.40			
		1.1 × 10 ⁸	7.09 (marginal)			
		1.0 × 10 ⁹	Deflagrated (3 min)			

DTA for irradiated HMX @ 20 °C/min^[185]:

Total dose (R)	Endotherms				Exotherms			
	1st		2nd		1st		2nd	
	Onset (°C)	Peak (°C)	Onset (°C)	Peak (°C)	Onset (°C)	Peak (°C)	Onset (°C)	Peak (°C)
0	192	199	271	272	272	286		
1.3×10^7	173	177	274	275	275	286		
1.1×10^8	185	190*			170	179	250	293
1.0×10^9	180	182			150	172	190	270

* = small dip

TGA for irradiated HMX^[185]:

Total dose (R)	Heating rate (°C/min)	Weight (mg)	Start of dec. (°C)	10% weight loss T (°C)	Total weight loss (%)	Remarks
0	20	8.4	250	282	10 @ 282 °C	Detonated @ 282 °C
1.3×10^7	20	10.9	180	266	15 @ 268 °C	Detonated @ 268 °C
1.1×10^8	20	8.2	55	250	21 @ 274 °C	Detonated @ 274 °C
1.0×10^9	20	8.2	105	185	14 @ 252 °C	Detonated @ 252 °C
0	50	10.3	275	–	23 @ 297 °C	Detonated @ 297 °C
0	80	9.5	280	–	6 @ 300 °C	Detonated @ 300 °C

Effect of gamma radiation on the mpt. and color^[185]:

Total dose (R)	Mpt. (°C)	Color
0	273.5	White
1.3×10^7	271.0	White
1.1×10^8	271.0	White
1.0×10^9	255 Dec.	White

IS for irradiated explosives, 50% fire height in in, Bruceton method (P.A. apparatus, 2 kg mass)^[185]:

Total Co ⁶⁰ gamma dose (R)	\bar{X} mean (in)	σ std. dev. (in)
0	14.04	1.04
1.3×10^7	11.04	1.44
1.1×10^8	8.96	2.57
1.0×10^9	9.96	2.40

Effect of gamma radiation on explosion T (5 s explosion T in °C) and activation energy (kcal/mol)^[185]:

Total dose (R)	5 s explosion T (°C)	Apparent activation energy (kcal/mol)
0	300	14.45
1.3×10^7	290	16.36
1.1×10^8	286	23.50
1.0×10^9	201	6.10

Effect of gamma radiation on rates of detonation^[185]:

Total dose (R)	Density (g/cc)	Density after irradiation (g/cc)	Rate of detonation (m/s)	Detonation pressure (kbar)
0	1.75	—	8,620	325
0.1×10^7	1.75	1.75	8,620	325
3×10^8	1.74	1.66	8,410	293
1.1×10^9	Pellets crumbled			

Refractive index	Data from ^[17] :				
	Face	HMX polymorph			
		α	β	γ	δ
	Alpha	1.561–1.565	1.589	1.537	-
	Beta	1.562–1.566	1.594–1.595	1.585	-
	Gamma	1.729–1.740	1.730–1.773	1.666	1.566
	Epsilon	-	-	-	1.607
	Omega	-	-	-	
Wedge test results	Data from ^[17] :				
	Density (g/cm ³)	Distance, x^* , to detonation (mm)		Pressure range (GPa)	
	1.891	$\log P = (1.18 \pm 0.02) \cdot (0.59 \pm 0.03)$ $\log x^*$, where P = pressure in GPa		4.41 < P < 9.55	

Fig. 16 data from^[153]:

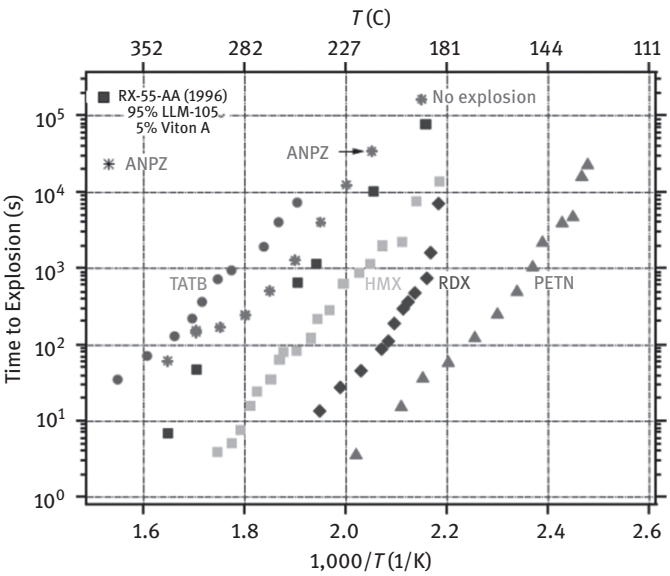


Fig. 16: ODTX results of ANPZ and TATB, HMX, RDX and PETN^[153].

	Octogen (β -HMX) ^[31, 41, 131, 174]	α -HMX ^[16, 18, 22, 35, 130, 174]	β -HMX ^[16, 18, 22]	γ -HMX ^[16, 22, 35, 41, 131]	δ -HMX ^[32, 174]	β -HMX ^[42, 43]
	Neutron diffraction	(HMX-II)	(HMX-I)	(HMX-III)*	(HMX-IV)	
Chemical formula	$C_4H_8O_8N_8$	$C_4H_8O_8N_8$	$C_4H_8O_8N_8$		$C_4H_8O_8N_8$	$C_4H_8O_8N_8$
Molecular weight [g mol ⁻¹]	296.18	296.18	296.18		296.18	296.18
Crystal system		Orthorhombic	Monoclinic	Monoclinic	Hexagonal	Monoclinic
Space group		Fdd2	$P 2_1 / c$ (no. 14)	$Pc, P 2 / c$ or $P 2 / n$	$P6_1$ or $P6_5$	$P 2_1 / n$
a [Å]	6.54	15.14	6.54	10.95	7.711(2)	6.5209(2)
b [Å]	11.05	23.89	11.05	7.93	7.711(2)	10.7610(2)
c [Å]	8.70	5.91	8.70	14.61	32.553(6)	7.3062(2)
α [°]	90	90	90	90	90	90
β [°]	124.3	90	102.8 ^[18] , 103 ^[22]	119.4	90	102.058(2)
γ [°]	90	90	90	90	120	90
V [Å ³]				1,105.25 ^[35]	1,676.3	501.37
Z	2	8	2	4	6	2
ρ_{calc} [g cm ⁻³]	1.894	1.838 ^[18] , 1.87 ^[22] 1.84087 ^[35]	1.902 ^[18] 1.96 ^[22]	1.78, 1.7798 ^[35]	1.586	1.962
T [K]			298 ^[22]	298 ^[22]	RT	20
	Unit cell constants of Eiland and Pepinsky are used			*It has been shown that γ -HMX is in fact a hydrate – $2C_4H_8N_8O_8 \cdot 1/2 H_2O$ ^[41]		

	β -HMX ^[43]	β -HMX ^[35]	γ -HMX ^[32, 35, 41]	δ -HMX ^[16, 35, 41]	β -HMX ^[100]	δ -HMX ^[100]	ϵ -HMX ^[100]
Chemical formula	C ₄ H ₈ O ₈ N ₈	C ₄ H ₈ O ₈ N ₈		C ₄ H ₈ O ₈ N ₈			
Molecular weight [g mol ⁻¹]	296.18	296.18		296.18	296.18	296.18	296.18
Crystal system	Monoclinic	Monoclinic	Monoclinic		Monoclinic	Hexagonal	Monoclinic
Space group	$P2_1/n$	$P2_1/c$ (no. 14)	Pc	$P6_3$ or $P6_1$			$P2_1/c$
a [Å]	6.5250(2)	6.5380(8)	13.271	7.711(2)	6.50	7.66	21.799
b [Å]	10.8249(2)	11.054(2)	7.90	7.711(2)	10.93	7.66	10.913
c [Å]	7.3175(1)	8.702(2)	10.95	32.553(6)	7.32	32.49	10.819
α [°]	90	90	90	90	90	90	90
β [°]	102.256(1)	124.44	106.8	90	103.3	90	97.43
γ [°]	90	90	90	120	90	120	90
V [Å ³]	505.07	518.668	1,099.01	1,676.27			
Z	2	2	4	6			10
ρ_{calc} [g cm ⁻³]	1.948	1.8963	1.82	1.76026	1.902	1.763	1.919
T [K]	120						
			*It has been shown that γ -HMX is in fact a hydrate – $2C_4H_8N_8O_8 \cdot 1/2H_2O$ ^[41]				

The cell constants reported in reference below are not a γ -form of HMX, but instead correspond to those of the hemihydrate^[174]; There are over 100 stoichiometric compounds which have been prepared between HMX and organic molecules^[174]; β -HMX can be prepared from a number of routes, for example, by very slow cooling of acetic acid, acetone, nitric acid or nitromethane solns.^[174] α -HMX can be prepared from the same solns. but with rapid cooling^[174], γ -HMX can be obtained by even more rapid cooling^[174], δ -HMX obtained rapidly chilling of, or pouring onto ice solns. in which it has slight solubility^[174]

	HMx ^[174, 175]	HMx ^[174, 176]	HMx ^[177]	HMx ^[177]	HMx ^[177]	HMx ^[177]
Chemical formula	C ₄ H ₈ O ₈ N ₈	C ₄ H ₈ O ₈ N ₈	C ₄ H ₈ O ₈ N ₈	C ₄ H ₈ O ₈ N ₈	C ₄ H ₈ O ₈ N ₈	C ₄ H ₈ O ₈ N ₈
Molecular weight [g mol ⁻¹]	296.18	296.18	296.18	296.18	296.18	296.18
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	<i>P</i> 2 ₁ / <i>c</i> (no. 14)	<i>P</i> 2 ₁ / <i>n</i> (no. 14)	<i>P</i> 2 ₁ / <i>n</i> (no. 14)	<i>P</i> 2 ₁ / <i>n</i> (no. 14)	<i>P</i> 2 ₁ / <i>n</i> (no. 14)	<i>P</i> 2 ₁ / <i>n</i> (no. 14)
<i>a</i> [Å]	6.540	6.533(1)	6.5289(5)	6.5245(10)	6.5254(9)	6.5255(10)
<i>b</i> [Å]	11.050	7.351(2)	10.9875(9)	11.0240(17)	10.9702(16)	11.0369(18)
<i>c</i> [Å]	8.700	11.032(3)	7.3453(5)	7.3619(11)	7.3503(11)	7.3640(12)
α [°]	90	90	90	90	90	90
β [°]	124.30	90	102.616(4)	102.642(9)	102.582(9)	102.670(10)
γ [°]	90	77.32(2)	90	90	90	90
<i>V</i> [Å ³]	519.387	516.88	514.20(7)	516.68(14)	513.53(13)	517.45(14)
<i>Z</i>	2	2	2	2	2	2
ρ_{calc} [g cm ⁻³]	1.894	1.903	1.913	1.904	1.915	1.901
<i>T</i> [K]	295	295	273	293	248	303

	HMX ^[175]	HMX ^[176]	HMX ^[177]	HMX ^[178]	γ -HMX ^[174, 179]	α -HMX ^[17]	β -HMX ^[17]	γ -HMX ^[17]	δ -HMX ^[17]
Chemical formula	C ₄ H ₈ O ₈ N ₈	C ₄ H ₈ O ₈ N ₈	C ₄ H ₈ O ₈ N ₈	C ₄ H ₈ O ₈ N ₈	2C ₄ H ₈ N ₈ O ₈ · ¹ / ₂ H ₂ O				
Molecular weight [g mol ⁻¹]	296.18	296.18	296.18	296.18	296.18	296.18	296.18	296.18	296.18
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic				
Space group	<i>P</i> 2 ₁ / <i>c</i> (no. 14)	<i>P</i> 2 ₁ / <i>n</i> (no. 14)	<i>P</i> 2 ₁ / <i>n</i> (no. 14)	<i>P</i> 2 ₁ / <i>c</i> (no. 14)	<i>Pn</i> (no. 7)				
<i>a</i> [Å]	6.5334(9)	6.5206(9)	6.5288(8)	21.799(3)	13.27(1)	15.14	6.54	10.95	7.66
<i>b</i> [Å]	10.9419(14)	10.9123(16)	10.8862(13)	10.913(2)	7.90(1)	23.89	11.05	7.93	-
<i>c</i> [Å]	7.3421(10)	7.3395(11)	7.3304(9)	10.819(2)	10.95(1)	5.91	7.37	14.61	32.49
α [°]	90	90	90	90	90				
β [°]	102.491(2)	102.467(9)	102.365(2)	97.43(2)	106.8(1)	-	102.8	119.4	
γ [°]	90	90	90	90	90				
<i>V</i> [Å ³]	512.45(12)	509.93(13)	508.91(11)	2552.15	1098.93				
<i>Z</i>	2	2	2	10	2	8	2	4	6
ρ_{calc} [g cm ⁻³]	1.919	1.929	1.933	1.927	1.817				
<i>T</i> [K]	223	198	173	200	295				

Effect of bead milling on results of Rietveld analysis^[99]:

Time of milling (h)	<i>a</i> (Å)	<i>b</i> (Å)	<i>c</i> (Å)	β (°)	Vol. (Å ³)
0	6.5552	11.0331	8.7085	124.422	519.55
1.0	6.5370	11.0425	8.7049	124.420	518.34
5.9	6.5389	11.0407	8.7000	124.442	517.99

Preparation of different HMX polymorphs using solvents^[16]:

Polymorph obtained	Conditions
α -HMX	Precipitated from the same solns. as for β -HMX but with more rapid cooling
β -HMX	Precipitated from a soln. of HMX in acetic acid, acetone, nitric acid or nitromethane with slow cooling
	α -HMX converted to β -HMX by cryst. from boiling acetone, acetonitrile or cyclohexanone
γ -HMX	Precipitated from the same solns. as for α - and β -HMX but with even more rapid cooling
δ -HMX	Crystallized from solns. such as acetic acid or betachloroethyl phosphate in which HMX shows low solubility, with very rapid cooling (e.g. by pouring over ice)

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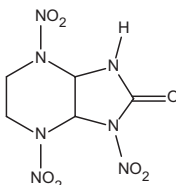
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6-Oxo-2,5,7-trinitro-2,5,7,9-tetraazabicyclo[4.3.0]nonane-8-one

Name [German, acronym]: 2,5,7-Trinitro-2,5,7,9-tetraazabicyclo
[4.3.0]nonane-8-one, [K-56]

Main (potential) use: Investigated as possible RDX replacement^[5]

Structural formula: high explosive



	HK-56		
Formula	$C_5H_7N_7O_7$		
Molecular mass [g mol ⁻¹]	277.15		
Appearance at RT	White powder ^[4] , white microcrystals (recryst. from CH ₃ CN) ^[4]		
IS [J]	35 cm ^[5]		
FS [N]	>360 ^[5]		
ESD [J]	0.0829 ^[5]		
N [%]	35.38		
Ω(CO ₂) [%]	-37.52		
T _{m,p.} [°C]	Dec. without melting ^[2] , 187–198 ^[4]		
T _{dec.} [°C]	201.55 (exo, onset), 203.75 (exo, peak max) (DSC @ 10 °C/min, N ₂ , hermetic pan, pinhole) ^[2] , 202.56 (exo, onset), 206.91 (exo, peak max) (DSC @ 10 °C/min, N ₂ , standard pan) ^[2]		
ρ [g cm ⁻³]	1.84 ^[1] , 1.84 (crystal) ^[4]		
Heat of formation	100.6 kJ/mol ^[5]		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
-Δ _{ex} U° [kJ kg ⁻¹]			
T _{ex} [K]		2,916 (@ 1.85 g cm ⁻³ , ΔH _f = -129.9 kJ/mol, calcd., JAGUAR) ^[3]	

p_{C-1} [kbar]		31.2 GPa (@ 1.85 g cm ⁻³ , $\Delta H_f = -129.9$ kJ/mol, calcd., JAGUAR) ^[3] 32.82 GPa (calcd., CHEETAH 7.0) ^[5]	
VoD [m s ⁻¹]		8,380 (@ 1.85 g cm ⁻³ , $\Delta H_f = -129.9$ kJ/mol, calcd., JAGUAR) ^[3] 8,628 (@ 1.85 g cm ⁻³ , calcd., CHEETAH 7.0) ^[5]	
V_0 [L kg ⁻¹]			
Vacuum stability test [cm ³ /h]	STANAG 4147 test 1B, total gas evolved after 40 h @ 100 °C, values in cc): 0.2857 ^[5]		
Vapor pressure [Pa]	1.52 × 10 ⁻¹² Torr @ 25 °C (est.) ^[2, 5] , 1.13 × 10 ⁻⁹ Torr @ 70 °C (est.) ^[2, 5] , 2.35 × 10 ⁻⁷ Torr @ 100 °C ^[2, 5]		
Solubility [g/mL]	5.1 × 10 ⁻¹ mg/mL (H ₂ O solubility @ 25 °C (measured)) ^[2]		
Compatibility	VTS compatibility (STANAG 4147 test 1B, 2.5 g of compound 1 mixed with 2.5 g of compound 2, total gas evolved after 40 h @ 100 °C, values in cc) ^[5] : 0.4146 (TNBA), 0.1175 (DNMT), – (PiPE), 0.2971 (DNP), 0.4653 (DNGU), – (LLM-105), 0.226 (HMX) concluding that all are compatible with HK-56 ^[5]		
K_{ow}	$K_{ow} = 0.016$ ^[2] , log $K_{ow} = -1.8$ ^[2] , $K_d = 0.92$ ^[2]		
K_{oc}	$K_{oc} = 40.3$ (measured) ^[2] , log $K_{oc} = 1.61$, $K_{oc} = 61.5$ (predicted) ^[2]		
ΔH_{vap} [kJ/mol]	147.3 (est.) ^[5]		

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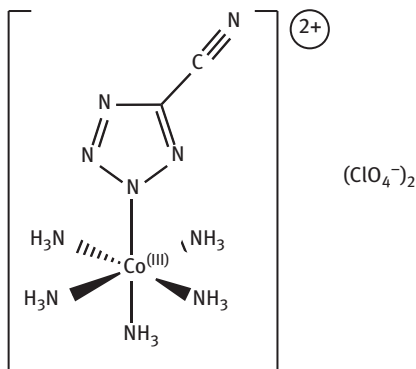
P

Pentaammine(5-cyanotetrazolato-*N*2)cobalt(III) perchlorate

Name [German, acronym]: (5-Cyanotetrazolato-*N*²)pentaamminecobalt(III) perchlorate, 2-(5-cyanotetrazolato) pentaamminecobalt(III) perchlorate [pentaammin (5-cyanotetrazolato-*N*2)cobalt(III) perchlorat, CP]

Main (potential) use: Applications in down hole completion work for the oil industry^[1, 2], defense^[1], exploding bridgewire (EBW) detonator for applications which require a hermetically sealed detonator^[2], CP as safer replacement for LA in low-voltage detonators^[3], primary explosive in safe blasting caps and safe commercial detonators^[5], possible replacement for primary explosives in hot-wire detonators^[6], secondary explosive^[8], for applications involving deflagration-to-detonation transition^[8], low voltage, hot-wire detonators^[8]

Structural formula:



	CP
Formula	C ₂ H ₁₅ CoN ₁₀ Cl ₂ O ₈
Molecular mass [g mol ⁻¹]	436.98
Appearance at RT	Free-flowing yellow-orange powder ^[6] , yellow free-flowing crystalline solid ^[7] , yellow solid ^[8, 10] , yellow-orange solid ^[11]

IS [J]	100–140 kg cm (drop height) ^[2] , ~40 cm (loose powder, 2 kg mass) ^[8] IS of CP solns. (0.5 M in DMSO, Olien-Mathieson apparatus, 5 kg mass, 0.2–0.3 mL soln., nonhermetic sealed Al pan in brass cup on anvil of apparatus) ^[9] : no ignitions in 20 attempts ^[9] $DH_{50} = 60.6 \pm 1.0$ cm(@ 68°F, 56% RH, ERL type 12 apparatus, type 12A tool, 2.5 kg mass, 35 mg sample, powder sample on Carborundum 120 flint paper, Bruceton up–down method) ^[10] DH_{50} (cm): 19 (fine) ^[10] , 9 (coarse) ^[10] , 61 ^[10]																					
FS [N]	1–1.5 kg (BAM) ^[2] , 1/10 goes @ 1.0 kg (@ 68°F and 60% RH, 0.031 cm ² contact area, BAM) ^[10] , Data from ^[10] : <table><tr><td>Test</td><td>CP, literature</td><td>CP values from^[10]</td></tr><tr><td rowspan="2">Friction (fine)</td><td>30 psig @ 8 ft/s</td><td>455 psig @ 0.1 ft/s</td></tr><tr><td>180 psig @ 3 ft/s</td><td></td></tr><tr><td rowspan="2">Friction (coarse)</td><td><30 psig @ 8 ft/s</td><td></td></tr><tr><td>420 psi @ 3 ft/s</td><td></td></tr></table>	Test	CP, literature	CP values from ^[10]	Friction (fine)	30 psig @ 8 ft/s	455 psig @ 0.1 ft/s	180 psig @ 3 ft/s		Friction (coarse)	<30 psig @ 8 ft/s		420 psi @ 3 ft/s									
Test	CP, literature	CP values from ^[10]																				
Friction (fine)	30 psig @ 8 ft/s	455 psig @ 0.1 ft/s																				
	180 psig @ 3 ft/s																					
Friction (coarse)	<30 psig @ 8 ft/s																					
	420 psi @ 3 ft/s																					
ESD [J]	>25 kV (Sandia Man Model testers) ^[2] , insensitive in bulk form but sensitive in confined pressed state ^[3] , spark sensitive as loose powder ^[1] , >20 kV @ 600 pF and 500 ohms (loose powder and unconfined pellet) ^[8, 10] , spark sensitivity increases with increasing density up to 1.6 g cm ⁻³ , but at greater densities the spark sensitivity decreases with increasing density ^[9] <table><tr><td>CP ρ (g cm⁻³)^[9]</td><td>Lowest fire (kV) ^[9]</td><td>Highest no-fire (kV) ^[9]</td></tr><tr><td>1.3</td><td>10</td><td>8</td></tr><tr><td>1.43</td><td>3.5</td><td>5</td></tr><tr><td>1.5</td><td>3.8</td><td>5.5</td></tr><tr><td>1.63</td><td>4.3</td><td>6</td></tr><tr><td>1.7</td><td>6</td><td>10</td></tr><tr><td>1.8</td><td>12</td><td>16</td></tr></table> No rxns. (0/10) @ 10 kV (1 J) (@ 68 °C, 56% RH, modified electrical instruments services electrostatic discharge tester, samples loaded into teflon washers, covered with 1 mm thick Mylar tape, sample $\rho = 1.4$ g cm ⁻³) ^[10] ESD threshold (J) ^[10] : 0.165 (fine) ^[10] , 0.326 (coarse) ^[10] , >1.0 ^[10]	CP ρ (g cm ⁻³) ^[9]	Lowest fire (kV) ^[9]	Highest no-fire (kV) ^[9]	1.3	10	8	1.43	3.5	5	1.5	3.8	5.5	1.63	4.3	6	1.7	6	10	1.8	12	16
CP ρ (g cm ⁻³) ^[9]	Lowest fire (kV) ^[9]	Highest no-fire (kV) ^[9]																				
1.3	10	8																				
1.43	3.5	5																				
1.5	3.8	5.5																				
1.63	4.3	6																				
1.7	6	10																				
1.8	12	16																				
N [%]	32.05																					
$\Omega(\text{CO}_2)$ [%]																						
$T_{\text{m.p.}}$ [°C]	Dec. occurs without melting ^[4]																					

$T_{\text{dec.}} [^{\circ}\text{C}]$	Dec. occurs without melting ^[4] , ~260 (endo, dissociation of NH_3 ligands from Co(III) center, DSC @ 5 $^{\circ}\text{C}/\text{min}$) ^[4] , 250 (weight loss begins and accelerates sharply @ 260 $^{\circ}\text{C}$, TGA) ^[4] , dec. on attempts to sublime under vacuum ^[4] , ~295 (exo peak max., DSC @ 10 $^{\circ}\text{C}/\text{min}$, open sample) ^[8] , 270 (onset, weak endo, stage 1 dec.) ~320 (exothermic peak max., broad, stage 2 dec.), ~345 (exo peak max., sharp, stage 3 dec.) (DSC @ 10 $^{\circ}\text{C}/\text{min}$, hermetically sealed) ^[8] , dec. is complex and shows autocatalysis characteristics ^[12]		
$\rho [\text{g cm}^{-3}]$	1.952 (crystal, X-ray@ RT) ^[1] , 1.989 (measured, pycnometer) ^[1] , 0.6 (loose powder) ^[6] , 1.97 (crystal) ^[7] , 1.974 (X-ray) ^[8, 10] , 1.96 (He pycnometer) ^[8, 11] , 1.989 (observed) ^[9]		
Heat of formation			
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^{\circ} [\text{kJ kg}^{-1}]$			
$T_{\text{ex}} [\text{K}]$			
$p_{\text{C-1}} [\text{kbar}]$			22.0 GPa (@ 1.52 g cm^{-3} , VISAR system, steel casing, initiated by RP-2 detonator) ^[9] 27.5 GPa (@ 1.77 g cm^{-3} , VISAR system, steel casing, initiated by RP-2 detonator) ^[9]
VoD [m s^{-1}]			CP requires fairly long column lengths (4–6 mm) in steel confinement to achieve steady-state detonation ^[2] $6.03 \pm 0.18 \text{ km/s}$ (@ 1.52 g cm^{-3} , VISAR system, steel casing, initiated by RP-2 detonator) ^[9] $6.79 \pm 0.09 \text{ km/s}$ (@ 1.77 g cm^{-3} , VISAR system, steel casing, initiated by RP-2 detonator) ^[9]
$V_0 [\text{L kg}^{-1}]$			
Critical explosion $T [^{\circ}\text{C}]$	508 K (cylindrical pellets, 0.238 mm radii, 1.5 g cm^{-3} nominal density, ARC, isothermal) ^[12] , ~450 K (slab pellets, 2.0 mm charge radius) ^[12] , ~460 K (cylinder pellets, 2.0 mm charge radius) ^[12] , ~475 K (sphere pellets, 2.0 mm charge radius) ^[12] , ~465 K (slab pellets, 1.0 mm charge radius) ^[12] , ~475 K (cylinder pellets, 1.0 mm charge radius) ^[12] , ~485 K (sphere pellets, 1.0 mm charge radius) ^[12] , ~482 K (slab pellets, 0.5 mm charge radius) ^[12] , ~495 K (cylinder pellets, 0.5 mm charge radius) ^[12] , ~500 K (sphere pellets, 0.5 mm charge radius) ^[12]		
5 s explosion $T [^{\circ}\text{C}]$ Autoignition $T [^{\circ}\text{C}]$	290 (DSC @ 10 $^{\circ}\text{C}/\text{min}$, sealed hermetic pans and cups) ^[2] , 340 (instantaneous autoignition) ^[6]		

Thermal stability	<p><0.05% reaction occurred after aging @ temperature up to 80 °C for 15 years^[2], stable for at least 100 h @ 160 °C^[2]</p> <p>Calcd. dec. products after 25 years @ two temperatures and corresponding accelerated aging times^[4]:</p>				
	Quantity determined	Dec. product produced in 25 years (mg x/g CP present initially)		Times equivalent @ 150 °C (h)	
		@ 30 °C	@ 70 °C	25 years @ 30 °C	25 years @ 70 °C
	Co ²⁺	2.76×10^{-7}	1.66×10^{-3}	1.4×10^{-4}	0.81
	NH ₄ ⁺	6.93×10^{-8}	6.23×10^{-4}	6.1×10^{-5}	0.55
	Cl ⁻	1.01×10^{-6}	2.72×10^{-3}	1.0×10^{-3}	2.7
	CN ⁻	4.56×10^{-13}	9.05×10^{-8}	3.4×10^{-8}	0.0067
	Gas evolution	1.01×10^{-3}	1.36	5.9×10^{-3}	7.9
<p>No dec. on storing @ 80 °C for 3 years (using Co(II) as the prime stability measurement, hermetically sealed detonator)^[8], ~2.2% rxn. on storing @ 120 °C for 3 years (using Co(II) as the prime stability measurement, hermetically sealed detonator)^[8], stable on storing <70 °C^[8], dec. in <612 days @ 120 °C (using Co(II) as the prime stability measurement, hermetically sealed detonator)^[8], little dec. of powder @ 80 °C^[9]</p> <p>Co²⁺ analysis of CP removed from aged minidets.^[8]:</p>					
	Environment	ppm Co ²⁺ present after aging			
		612 days	795 days	1,078 days	
	RT	166	301	456 ± 215	
		334	630	778 ± 209	
		<100			
		<100			
	60 °C	254	383	639 ± 169	
		<100	355	1,370 ± 134	
		313			
	80 °C	299	461	463 ± 93	
		824	542	839 ± 171	
	120 °C	3,710	3,070	3,160 ± 218	
		2,270	4,557	4,180 ± 138	
		2,700			
		3,150			

	Aging studies @ ≤ 80 °C for 3 years show that formation of Co(II) is nominally <800 ppm, not significantly greater than @ RT ^[11] but ~2.5% conversion @ 120 °C ^[11]																					
Burn rate [mm/s]	0.4–0.5 km/s (for column lengths of 1.6–2.4 mm) ^[9] , 0.932 km/s (terminal velocity @ 1.42 g cm ⁻³) ^[9] , 1.035 km/s (terminal velocity @ 1.62 g cm ⁻³) ^[9]																					
Solubility [g/mL]	Soluble in DMSO ^[9]																					
Hygroscopicity	Nonhygroscopic ^[5] , slightly hygroscopic ^[6] , 0.15 w/o @ RT @ 95% RH ^[8] , 0.12–0.27% moisture uptake ^[11]																					
Photosensitivity	Crystals are radiation sensitive (Mo-K α , $\lambda = 0.71069$ Å) ^[11] , mounted crystals are stable but rapidly degrade after several days exposure to X-ray radiation ^[11]																					
Compatibility	Compatible with all typical hot wire and EBW materials of construction except Cu and Zn and their alloys ^[2] , incompatible with Ag and Au ^[2] , compatible with epoxy adhesives ^[2, 8] , incompatible with Cu ^[8] , compatible on mixing with boron/calcium chromate and pressed with Trophet A and Kovar wires after 8 months @ 50% and 92% RH and up to 120 °C ^[8] , incompatible with Cu (corrosion) ^[8] , compatible with Alumina ^[8] , Amine and anhydride cured epoxy are compatible (CRT, 4 months, 120 °C) ^[8] , compatible with most metallic, ceramic and epoxy materials used in typical detonator designs ^[8] , no corrosive attack on Alumina, Kovar or Nichrome (SEM) ^[11]																					
Plate dent test	0.45 mm (steel witness plate dent) ^[2]																					
Flying plate velocity [mm/us]	2.7 ^[2]																					
Shock sensitivity	Insensitive in bulk form, sensitive in unconfined pressed state ^[3]																					
Hot-wire sensitivity	Does not sustain in bulk form but sustains detonation in confined pressed state ^[3]																					
Coefficient of thermal expansion [mm/mm°C]	<p>60 × 10⁻⁶ (@ 25–50 °C)^[8, 10], 52 × 10⁻⁶ mm/mm-°C @ -50 – -25 °C^[11], 66 × 10⁻⁶ mm/mm-°C @ 100–125 °C^[11], 60 × 10⁻⁶ mm/mm-°C @ RT^[11]</p> <p>CP CTE values, α, $\mu\text{m}/\text{m}^\circ\text{C}$, data from TMA method (sample length = 0.089 cm, sample diameter = 0.508 cm, mass = 0.306 g, sample volume = 0.0180 cc, sample $\rho = 1.696$ g/cc)^[10]:</p> <table><tr><td>Material</td><td>-20 °C -0 °C</td><td>0 °C -25 °C</td><td>25 °C -50 °C</td><td>50 °C -75 °C</td><td>75 °C -100 °C</td><td>100 °C -125 °C</td></tr><tr><td>Ref^[10] results</td><td>59</td><td>55</td><td>59</td><td>56</td><td>55</td><td>62</td></tr><tr><td>Lit. values^[10]</td><td>58</td><td>59</td><td>60</td><td>62</td><td>66</td><td>71</td></tr></table>	Material	-20 °C -0 °C	0 °C -25 °C	25 °C -50 °C	50 °C -75 °C	75 °C -100 °C	100 °C -125 °C	Ref ^[10] results	59	55	59	56	55	62	Lit. values ^[10]	58	59	60	62	66	71
Material	-20 °C -0 °C	0 °C -25 °C	25 °C -50 °C	50 °C -75 °C	75 °C -100 °C	100 °C -125 °C																
Ref ^[10] results	59	55	59	56	55	62																
Lit. values ^[10]	58	59	60	62	66	71																

Heat capacity [cal/g°K]	0.1545 + 0.0003 (@ 353–453 K) ^[8, 10, 11]
Laser ignition sensitivity	50% initiation threshold = 0.03 J/mm ² (Ruby laser) ^[11] , no-fire level = 0.01 J/mm ² (Ruby laser) ^[11] , initiation threshold = 0.25 J/mm ² (neodymium laser, 1.0 mm diameter, 630 μs pulse) ^[11]
Hot-wire ignition sensitivity	Mean all-fire energy (kerGs)/ρ (g cm ⁻³) ^[11] : ~18 kerGs @ 1.6 g cm ⁻³ (43–88 μm particle size) ^[11] , ~21 kerGs @ 1.6 g cm ⁻³ (53–90 μm particle size) ^[11] , ~20 kerGs @ 1.7 g cm ⁻³ (88–246 μm particle size) ^[11]

Temperature and total energy to bridgewire at CP ignition, data from ^[9]:

Avg. power to bridgewire ~150 W	Parameter	Avg. power to bridgewire ~5,500 W
1.46	CP density, Mg/m ³	1.42
195 ± 10	Ignition time, μs	13 ± 1
578 ± 10	Bridgewire temp., K	983 ± 10
25 ± 1	IE at ignition, mJ	59 ± 6
1.55	CP density, Mg/m ³	1.62
172 ± 5	Ignition time, μs	10 ± 1
554 ± 10	Bridgewire temp., K	995
23 ± 1	IE at ignition, mJ	47 ± 5

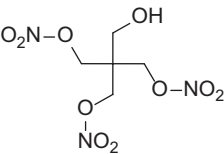
	CP ^[1]	CP ^[8, 10]	CP ^[9, 11]
Chemical formula	C ₂ H ₁₅ CoN ₁₀ Cl ₂ O ₈	C ₂ H ₁₅ CoN ₁₀ Cl ₂ O ₈	C ₂ H ₁₅ CoN ₁₀ Cl ₂ O ₈
Molecular weight [g mol ⁻¹]	437.04	437.04	437.04
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	<i>P</i> 2 ₁ / <i>a</i>		<i>P</i> 2 ₁ / <i>a</i>
<i>a</i> [Å]	24.813(5)		24.777(9)
<i>b</i> [Å]	7.661(2)		7.673(3)
<i>c</i> [Å]	7.971(1)		7.884(3)
α [°]	90		90
β [°]	101.17(1)		101.20(1)
γ [°]	90		90
<i>V</i> [Å ³]	1,486.5		
<i>Z</i>	4		4

ρ_{calc} [g cm ⁻³]	1.952	1.974	1.974
T [K]	RT		
Miscellaneous	Crystals obtained from aq. soln.		

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Pentaerythritol trinitrate

Name [German, acronym]: Pentaerythritol trinitrate [pentaerythrittrinitrat, PETRIN]
Main (potential) use: Ingredient in explosives, propellants or igniters^[4], intermediate in the preparation of many mixed nitrate esters^[8, 10], explosive, propellant or low mpt. components in gunpowder^[11]
Structural formula:



	PETRIN		
Formula	C ₅ H ₉ N ₃ O ₁₀		
Molecular mass [g mol ⁻¹]	271.14		
Appearance at RT	Viscous liquid ^[8] , white solid ^[11]		
IS [J]	2.49–4.98 (5–10 in, 2 kg mass, 38 mg sample, P.A.) ^[4] , 5–10 in (P.A.) ^[8] , lower than that of PETN ^[11] , 285 cm (some smoke, type 12A) ^[12] , 285 cm (no smoke at all, type 12B) ^[12] , 5–10 in (1 lb mass, P.A.) ^[8]		
N [%]	15.50		
Ω(CO ₂) [%]	–26.55		
T _{m.p.} [°C]	30 ^[1] , 26–28 ^[4, 11] , <20 (production grade) ^[8] , 26–28 (purified) ^[8] , 27–28 ^[10] , –28 (freezing point) ^[8]		
T _{b.p.} [°C]	130 (@ 4 mm Hg, dec.) ^[4]		
T _{dec.} [°C]	130 ^[4] , 130 (@ 4 mm Hg) ^[8]		
ρ [g cm ⁻³]	1.54 ^[4, 7, 11] , 1.54 (@ 20 °C) ^[8] , 1.632 (@ 293 K) ^[1]		
Heat of formation	–134 kcal/mol (ΔH _f @ 25 °C) ^[8] , –2,069 kJ/kg (enthalpy of form.) ^[7]		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
–Δ _{ex} U° [kJ kg ⁻¹]	5,218	5,037.54 kJ/kg ^[11]	5,038 ^[4] 5,230 [H ₂ O (l)] ^[7] 4,777 [H ₂ O (g)] ^[7] 1,204 cal/g ^[4, 8]
T _{ex} [K]	3,501		

p_{CJ} [kbar]	253		
VoD [m s ⁻¹]	7,777 (@ TMD)	7,380 (@ 1.54 g cm ⁻³ (TMD), calcd., R-P method) ^[9] 8,500 (@ 1.54 g cm ⁻³ (TMD), calcd., Aizenshtadt) ^[9] 7,610 (@ 1.54 g cm ⁻³ (TMD), calcd., K-J) ^[9]	7,640 (@ 1.54 g cm ⁻³) ^[3]
V_0 [L kg ⁻¹]	767		902 ^[5, 7] 918 ^[6]

5 s explosion T [°C] Explosion T [°C]	~280 (minimum explosion T , Wenograd test) ^[8]
Vacuum stability test [cm ³ /h]	2.54–5.65 cc/40 h @ 100 °C ^[4, 11]
Vapor pressure [atm. @ °C]	4.5×10^4 mm Hg @ 60 °C ^[8]
Viscosity [cP]	Absolute viscosity (poises): 14.8 @ 17 °C ^[4] , 4.8 @ 23 °C ^[4] , 3.0 @ 28 °C ^[4] , 1.2 @ 38 °C ^[4] Production grade: 14.8 @ 17 °C ^[8] , 4.8 @ 23 °C ^[8] , 3.0 @ 28 °C ^[8] , 1.2 @ 38 °C ^[8]
Dipole moment [D]	5.06 ^[8]

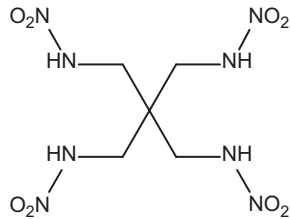
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Pentaerythrityl tetranitramine

Name [German, acronym]: 2,2-Bis(nitroaminomethyl)propane-1,3-dinitroamine, [PETNA]

Main (potential) use: high explosive

Structural formula:



	PETNA		
Formula	C ₅ H ₁₂ N ₈ O ₈		
Molecular mass [g mol ⁻¹]	312.23		
Appearance at RT	Colorless crystals ^[1, 2]		
IS [J]	6 (5 or 10 kg mass, 20 mg sample, BAM) ^[1]		
N [%]	35.89		
Ω(CO ₂) [%]	−41.00		
T _{m,p.} [°C]			
T _{dec.} [°C]	183 (DSC @ 10 °C/min, N ₂) ^[1, 2]		
ρ [g cm ⁻³]	1.778 (gas pycnometry @ 25 °C) ^[1, 2]		
Heat of formation	−0.193 kJ/g (Δ _f H ^o ₂₉₈) ^[1]		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
−Δ _{ex} U ^o [kJ kg ⁻¹]			
T _{ex} [K]			
p _{C-J} [kbar]		31.6 (@ 1.778 g cm ⁻³ , calcd., CHEETAH 5.0) ^[1, 2]	
VoD [m s ⁻¹]		8,657 (@ 1.778 g cm ⁻³ , calcd., CHEETAH 5.0) ^[1, 2]	
V ₀ [L kg ⁻¹]			

	PETNA ^[2]
Chemical formula	C ₅ H ₁₂ N ₈ O ₈
Molecular weight [g mol ⁻¹]	312.23
Crystal system	Tetragonal
Space group	<i>I</i> -4 (82)
<i>a</i> [Å]	9.6543(11)
<i>b</i> [Å]	9.6543(11)
<i>c</i> [Å]	6.3283(9)
α [°]	90
β [°]	90
γ [°]	90
<i>V</i> [Å ³]	589.83(13)
<i>Z</i>	2
ρ_{calc} [g cm ⁻³]	1.758
<i>T</i> [K]	293

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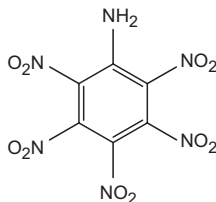
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Pentanitroaniline

Name [German, acronym]: 2,3,4,5,6-Pentanitroaniline, [pentanitroanilin, PNA]

Main (potential) use: secondary explosive

Structural formula:



	Pentanitroaniline									
Formula	C ₆ H ₂ N ₆ O ₁₀									
Molecular mass [g mol ⁻¹]	318.11									
Appearance at RT	Clear yellow plate crystals ^[1] , crystalline yellow solid ^[2]									
IS [J]	H ₅₀ = 0.15 m ^[4] , H ₅₀ = 15 cm ^[5] , H _{50%} = 22 cm (2.5 kg mass, type 12 tool, 35 mg sample in conical pile, 1 in ² garnet paper) ^[6] , H _{50%} = 22 cm (2.5 kg mass) ^[7]									
ESD [J]	Data from ^[3] : <table><tr><th colspan="3">50% point energy (J)</th></tr><tr><td>3 mil foil</td><td>10 mil foil</td><td>% expl.</td></tr><tr><td>0.21</td><td>0.31</td><td>75</td></tr></table>	50% point energy (J)			3 mil foil	10 mil foil	% expl.	0.21	0.31	75
50% point energy (J)										
3 mil foil	10 mil foil	% expl.								
0.21	0.31	75								
N [%]	26.42									
Ω(CO ₂) [%]	−15.09									
T _{m.p.} [°C]										
T _{dec.} [°C]	192–200 (dec.) ^[1] , 193–202 ^[1, 2] , 188–192 (recryst. from boiling 1,2-dichoroethane, some dec. occurred) ^[2] , 210–211 (chunky yellow crystals recryst. from benzene) ^[2]									
ρ [g cm ⁻³]	186 (obs.) ^[6]									

Heat of formation			
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^\circ$ [kJ kg ⁻¹]			
T_{ex} [K]			
$p_{\text{C-J}}$ [kbar]		366 (@ 1.92 g cm ⁻³ , calcd.) ^[6]	
VoD [m s ⁻¹]		8,810 (@ 1.92 g cm ⁻³ , calcd.) ^[6]	
V_0 [L kg ⁻¹]			

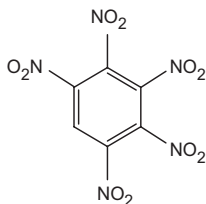
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Pentanitrobenzene

Name [German, acronym]: Pentanitrobenzene, [pentanitrobenzol, PNB]

Main (potential) use: high explosive

Structural formula:



	Pentanitrobenzene		
Formula	$\text{C}_6\text{H}_5\text{N}_5\text{O}_{10}$		
Molecular mass [g mol ⁻¹]	303.10		
Appearance at RT	Pale yellow crystalline needles ^[1]		
IS [J]	5 (BAM, 100–500 µm grain size) ^[1] , $H_{50\%} = 11$ cm (type 12 tool, 2.5 kg mass, 35 mg sample, garnet paper, B.M.) ^[2] , $H_{50\%} = 11$ cm (2.5 kg mass) ^[5]		
FS [N]	96 (BAM, 100–500 µm grain size) ^[1]		
ESD [J]	63 mJ (100–500 µm grain size) ^[1]		
N [%]	23.11		
$\Omega(\text{CO}_2)$ [%]	–13.2		
$T_{m,p.}$ [°C]	143 (onset, DTA @ 5 K/min) ^[1]		
$T_{dec.}$ [°C]	220 (DTA @ 5 K/min) ^[1]		
ρ [g cm ⁻³]	1.91 (recalculated for RT from LT X-ray) ^[1] , 1.910 (crystal @ 143 K) ^[1]		
Heat of formation	66.4 (ΔH_f , calcd., CBS-4M) ^[1] , –39.9 kcal/mol (ΔH_f (g) @ 25 °C, calcd., MINDO/3) ^[4]		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{ex}U^o$ [kJ kg ⁻¹]			
T_{ex} [K]			
p_{C-J} [kbar]		355 (@ 1.91 g cm ⁻³ , calcd.) ^[2] 38.96 GPa (@ 1.98 g cm ⁻³ , calcd., K-J) ^[3]	
VoD [m s ⁻¹]		8,700 (@ 1.91 g cm ⁻³ , calcd.) ^[2] 9,110 (@ 1.98 g cm ⁻³ , calcd., K-J) ^[3]	

V_0 [L kg ⁻¹]			
I_{sp} [s]	251 (calcd., EXPLO5 6.03, 70 kbar, isobaric combustion, equilibrium expansion) ^[1] , 259 (15% Al, calcd., EXPLO5 6.03, 70 kbar, isobaric combustion, equilibrium expansion) ^[1] , 234 (15% Al, 14% binder (6% polybutadiene acrylic acid, 6% polybutadiene acrylonitrile, 2% bisphenol A ether), calcd., EXPLO5 6.03, 70 kbar, isobaric combustion, equilibrium expansion) ^[1]		
Solubility [g/mL]	Recryst. from CH ₂ Cl ₂ ^[1]		
Compatibility	dec. in moist environment ^[1] , ~50% dec. in polar solvents (e.g. acetone) within 3 days ^[1]		
Dipole moment, μ [D]	2.90 (gas @ 25 °C, calcd., MINDO/3) ^[4] , 3.44 (gas @ 25 °C, calcd., MNDO) ^[4]		

	Pentanitrobenzene ^[1]
Chemical formula	C ₆ HN ₅ O ₁₀
Molecular weight [g mol ⁻¹]	303.10
Crystal system	Triclinic
Space group	<i>P</i> -1
<i>a</i> [Å]	8.1268(5)
<i>b</i> [Å]	13.1290(8)
<i>c</i> [Å]	20.3142(15)
α [°]	88.676(5)
β [°]	79.512(6)
γ [°]	81.601(5)
<i>V</i> [Å ³]	2,108.4(2)
<i>Z</i>	8
ρ_{calc} [g cm ⁻³]	1.910
<i>T</i> [K]	143
	recryst. from cold CH ₂ Cl ₂

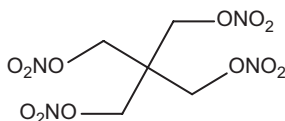
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PETN

Name [German, acronym]: Pentaerythritol tetranitrate, 2,2-bis[(nitrooxy)methyl]-1,3-propanediol dinitrate, penthrite, nitropenta, nyperite, pentyl, nitropentaerythrite, penta, pentryt, TEN (USSR) [pentrit, nitropentaerythrit, niperyth, nitropenta, NP, PETN][†]

Main (potential) use: Booster explosive, ingredient in grenades and small-caliber projectiles, in World War II: secondary explosive charge for filling grenades, detonating fuses, ammunition, explosive blends^[63], excellent transmitter of a detonation from initiating explosive to secondary explosive^[63], explosive core of detonating cords^[102], booster and detonator base charge^[102], ingredient of priming compositions^[107], in the manufacture of pentolite and other composite bursting charges^[107]

Structural formula:



[†] Phlegmatized (desensitized) PETN is prepared by adding 10% of montan wax (lignit) and often used due to the relatively high sensitivity of PETN^[63]

	PETN
Formula	$C_5H_8N_4O_{12}$
Molecular mass [g mol ⁻¹]	316.14
Appearance at RT	White crystalline substance ^[63, 10, 117, 138] , usually needles or column-shaped crystals ^[63] , cubic crystals obtained by recryst. from ethyl acetate ^[63] , crystallizes from H ₂ O as tetragonal crystals ^[64] , white solid ^[91] , fine crystalline or granular powder which is white (pure) or light gray (if impurities are present) ^[102] , white prismatic needles ^[107] , tetragonal crystals from normal manufacturing ^[20] , white or light buff solid ^[8] , crystal shape varies depending on solvent used during crystallization <i>e.g.</i> needle, bevel, stable α -cubic, unstable β -cubic ^[138]

IS [J]^[9]

3.59 (1st reaction)^[5, 31], 2.90 (sound)^[5, 31], 17 cm (3.34 J, 2 kg mass, B. M.)^[8, 9], 6 in (2.99 J), 2 kg mass, P. A.)^[8, 9], 3.34 cm (17 cm, 2 kg mass, 20 mg sample, B.M.)^[11–13], 15 cm (P.A.)^[11, 12], 2.99 (6 in, 2 kg mass, 16 mg sample, P.A.)^[13], 5.40 (E.R.L.)^[11, 12], 3–4.2^[17], $H_{50\%} = 13$ cm (US-NOL apparatus)^[35], $H_{50\%} = 13$ cm (2.5 kg hammer, 35 mg sample, US Naval lab)^[67], $H_{50} = 12$ cm (tool type 12)^[21], $H_{50} = 37$ cm (tool type 12B)^[21], $H_{50} = 11$ cm (tool type 12, 5 kg mass)^[26], $IS_{LL} = 0.5$ m^[24], $IS_{A50} = 0.9$ m^[24], median height = 66 cm (5 kg mass, 30 mg sample, Rotter apparatus)^[37], drop weight = 3.5 Nm^[39], Rotter Fol = 50^[43], US drop hammer = 12–15 cm^[43], $E_{dmin} = 2.5$ (BAM, 5 kg, max. level with six consecutive negative results)^[141], $H_{50} = 12$ cm^[59], 16 cm (NEDED)^[60], 14 cm (LANL)^[60], $H_{50\%} = 60$ –80 cm (500 g hammer)^[67], minimum hot-spot T for initiation by impact = 400–430 °C (in presence of grit)^[67], $H_{20\%} = 50$ cm (2 kg mass)^[68], $H_{50\%} = 60$ cm (2 kg mass)^[68], $H_{80\%} = 70$ cm (2 kg mass)^[68], 12 cm (Bruceton method, type 12 tool, 2.5 kg mass, 40 mg sample, 5/0 sandpaper, 25 trials)^[73], 6.5^[92], $Ed_{min} = 5$ (BAM, 5 kg mass, RT)^[94], $H_{50\%} = 12$ cm (2.5 kg mass, LANL type 12, PETN type RPS 3518)^[96], 1,422 mm (drop height, Rotter impact test)^[100], 1,555 mm (drop height, Rotter impact test, + 5% DETA)^[100], 60–80 cm (0.5 kg mass)^[105], 13 cm (max. height for no explosions, 5 kg mass)^[107], $DH_{50} = 25.2$ cm (4 kg mass, Bruceton method, 35 mg sample, 120 grit sandpaper, LLNL small-scale apparatus)^[109], 17 cm (2 kg mass)^[117], 6 in (16 mg sample, P.A.)^[119], 14 cm (50% point, type 12 tool, 2.5 kg mass, sandpaper)^[125], 16 cm (50% point, type 12 tool, 2.5 kg mass, sandpaper)^[125]

Powdered samples: $H_{50\%} = 12$ cm (NOL)^[37], $H_{50\%} = 12$ cm (LASL)^[37], $H_{50\%} = 43$ cm (B.M., ERL)^[37], $H_{10\%} = 17$ cm (P.A., B.M.)^[37], $H_{10\%} = 6$ cm (P.A.)^[37]

BAM (artificial aging performed as isothermal @ 70 °C for 113 days in absence of air or moisture): fresh PETN $E_{50} = 4.1$ ^[12]; aged PETN $E_{50} = 3.6$ ^[12], 50% explosion prob. = kinetic energy of 0.20 kg/cm²^[63], 20 cm but sometimes by a drop of 10–15 cm (2 kg mass, detonates)^[64]

Drop height = 1.05 m, sample thickness = 1.0–2.0 mm, drop weight = Al alloy plate of mass ~5.5 kg, impact velocity from max. drop height = ~4.5 ms⁻¹ producing max. impact pressure of ~1 GPa^[69]:

Material	Pellet diameter (mm)	ρ (% TMD)	No. of tests	% positive
Conventional PETN (powders, grain size = 10–200 μ m)	4	50–60	3	100
	8	63–68	3	100
	4	90–94	3	100
	8	80–85	3	100
Ultrafine PETN (powders, grain size = micron)	8	45–48	3	33
	4	90–94	3	33
	6	78–84	3	80
	8	73–77	3	33
	4	37–45	3	0

Drop height = 1.3 m, sample thickness = 1.0–2.0 mm, drop weight = Al alloy plate of mass ~5.5 kg^[69]:

Material	Pellet diameter (mm)	ρ (% TMD)	no. of tests	% positive
Conventional PETN (powders, grain size = 10–200 μm)	4	54–75	5	100
	6	48–50	3	100
	8	59–66	3	100
	4	90–94	5	100
	6	72–80	3	100
	8	84	3	100
Ultrafine PETN (powders, grain size = micron)	8	42–49	3	0
	4	72–92	21	10
	6	83–85	3	0
	8	74–78	3	0

$H_{50\%}$, up–down method, 25 mg samples, pressed to 10 kbar to give pellets of 5 mm diameter, 0.8 mm height; grit was fine, very fine or coarse where stated; PC = polycarbonate, PS = polysulfone, PMMA = polymethyl methacrylate, PP = polypropylene, HDPE = high-density polythene^[55]:

Sample (sample + binder)	50% height (cm)	Sample (sample + binder)	50% height (cm)
PETN (pure)	21.8 \pm 1.0	PETN + HDPE	24.8 \pm 1.5
PETN + PC (very fine)	10.5 \pm 2.0	PETN + PMMA (coarse)	21.0 \pm 1.6
PETN + PC (very fine, repeat)	10.7 \pm 0.6	PETN + PMMA (fine)	19.2 \pm 0.8
PETN + PS (very fine)	11.1 \pm 0.3	PETN + PP (very fine)	18.8 \pm 0.8
PETN + PS (fine)	13.0 \pm 1.5	PETN + PP (very fine, 10% grit)	19.2 \pm 0.7
PETN + PS (coarse)	10.4 \pm 0.6	PETN + polyester	15.5 \pm 1.0

Initiation of explosion by impact of PETN in the presence of grit^[119]:

Grit added	Impact explosion efficiency, %	Grit added	Impact explosion efficiency, %
Nil (pure PETN)	2	Silver iodide	–
AN	3	Borax	30
Potassium bisulfate	3	Bismuthinite	42
Silver nitrate	2	Glass	100
Sodium dichromate	0	Rock salt	6
Potassium nitrate	0	Chalcocite	50
Potassium dichromate	0	Galena	60
Silver bromide	6	Calcite	43
Lead chloride	27		

17 cm (2 kg mass)^[138], $H_{100\%} = 25$ cm (10 kg drop weight)^[138]

Rotter impact data: 27 mg sample, Bruceton method/25 drop run to obtain $H_{50\%}$; initiation criteria = 1 mL gas evolved or 0.5 mL accompanied by smoke or evidence of burning in the sample; data from^[139]:

Rotter impact data		US data	
F of I	Gas evolved (mL)	NSWC/NOL, ERL type 12	NWC B.M. type 12
50	12	12	12

$H_{50\%} = 16$ cm (4 kg mass, B.M. design 5)^[140], $H_{50\%} = 19$ cm (5 kg mass, plane sandblasted surfaces)^[140], 9 cm (sensitivity to glancing impact, Hercules sliding rod, sandblasted surfaces, 45° slide angle, 10 lb rod, 30 mg sample)^[140]

FS [N]

Crackles with steel shoe (friction pendulum test)^[13, 119], unaffected by fiber shoe (friction pendulum test)^[13], 80^[17], $P_{fr,LL} = 175$ MPa^[24], $P_{fr,50\%} = 345$ MPa^[24], $G_{min} = 60$ (BAM Julius-Peters, max. level with six consecutive negative runs)^[46], 70 Nm (50% value, BAM)^[58], 73 N (BAM, limiting load)^[65], 60 N (BAM, limiting load)^[65], $(H_{50}Wg)^{-1} = 3$ Nm^[66], rel. insensitive, but makes loud crackling when rubbed in rough porcelain mortar^[64], 35–40 cm (torpedo friction, 1 kg @ 80 °C, 0.5 m/s)^[67,105], 10 kg (friction wheel, 1 kg @ 80 °C, 0.5 m/s)^[67, 105], minimum hot-spot T for initiation by friction = 400–430 °C^[67], 18.6 kg load (20% samples fired, Julius-Peters)^[68], 19.2 kg (80% samples fired, Julius-Peters)^[68], 59^[92], $G_{min} = 60$ (BAM Julius Peters, max. level with six consec. negative runs)^[94], 9.6 kg (50% load, Bruceton method, BAM, PETN type RPS 3518)^[96], 60 kg (max. pressure for no explosions between two rubbing surfaces)^[107]

Rotary FS mean figure of friction (FoF) = 2.4^[25, 65], Rotary FoF = 1.3^[65], BAM mean limiting load = 73 N^[25]

Mallet friction test: steel on steel = 50%^[25], nylon on steel = 0%^[25], wood on softwood = 0%^[25, 127], wood on hardwood = 0%^[25, 127], wood on Yorkstone = 0%^[25], wood mallet on stone = 100%^[127]

BAM (artificial aging performed as isothermal @ 70 °C for 113 days in absence of air or moisture): fresh PETN F_{50} = 64^[12]; aged PETN F_{50} = 55^[12]

Gelled PETN with different PETN concentrations and different gels, CGC = critical gellator concentration, BAM, Bruceton method, FS measured 24 h after preparation, $E_{50\%}$ ^[97]:

Gel type	Gellant system	Solvent	CGC	PETN conc. [% v/v]	FS [N]	
–	–	Powdered	–	100	28	
Physical organic gels	GSSG	DMF	8.2 mM	21	220 ± 110	
Physical hydrogels	Guar gum	H ₂ O	0.035 g/mL	20	> 360	
	Xanthan gum	H ₂ O/EtOH	0.120 g/mL	50	> 360	
	1.5% w/w PAA	H ₂ O/ isopropanol	Not a solid gel	34	> 360	
				50	216	
				65	112	
	3.0% w/w PAA			50	> 360	
				65	235 ± 25	
				72	130 ± 50	
	Physical cross-linked hydrogel (Ionotropic gel)		1.5% PAA-Fe ³⁺	6.4 μM/mL	50	> 360
					65	120 ± 40
72					95	

	Initiation of explosion by friction of PETN in the presence of grit ^[119] :																						
	Grit added	Friction explosion efficiency, %	Grit added	Friction explosion efficiency, %																			
	Nil (pure PETN)	0	Silver iodide	100																			
	AN	0	Borax	100																			
	Potassium bisulfate	0	Bismuthinite	100																			
	Silver nitrate	0	Glass	100																			
	Sodium dichromate	0	Rock salt	50																			
	Potassium nitrate	0	Chalcocite	100																			
	Potassium dichromate	0	Galena	100																			
	Silver bromide	50	Calcite	100																			
	Lead chloride	60																					
	$H_{50\%} = 7.5$ cm (friction pendulum, 30 mg sample, sandblasted surface, 2 in ball, 5 kg weight, 8° angle of incidence) ^[140]																						
ESD [J]	0.06 (100 mesh, unconfined) ^[13] , 0.21 (100 mesh, confined) ^[13] , $E_{50} = 40$ mJ (PETN-I, crystal width ≤ 0.125 mm) ^[83] , $E_{50} = 139$ mJ (PETN-II, crystal width ≤ 0.500 mm) ^[83] , 56 mJ (old equipment, different particle sizes), >5,600 mJ (new equipment) ^[95] , 0.0625 (ABL, PETN type RPS 3518) ^[96] , 0.06 (unconfined) ^[119] , 0.21 (confined) ^[119] Spark sensitivity: 0.19 (brass electrode, 3 mm Pb foil thickness) ^[20, 21] , 0.36 (brass electrode, 10 mm Pb foil thickness) ^[20, 21] , 0.41 (steel electrode, 10 mm Pb foil) ^[20, 21] , 0.1 (steel electrode, 1 mm Pb foil) ^[20] , discharge energy increases with increasing PETN particle size, packing density, water content, circuit inductance and decreasing temperature ^[20] Max. nonignition energy = 0.036, max. nonignition spark voltage = 12,000 V (2.6 micron particle size, 0.005 in spark gap, 500 μ F capacitance) ^[20] Highest electrostatic discharge energy @ 5,000 volts for zero ignition probability ^[35] :																						
	<table> <tr> <th rowspan="2"></th><th colspan="2">Highest E for zero ignition probability</th><th colspan="2">Type of ignition</th></tr> <tr> <th>Confined</th><th>Unconfined</th><th>Confined</th><th>Unconfined</th></tr> <tr> <td>Bulk PETN</td><td>> 11.0</td><td>0.21</td><td>None</td><td>Deton.</td></tr> <tr> <td>PETN through 100 mesh</td><td>0.062</td><td>0.21</td><td>Deflag.</td><td>Deton.</td></tr> </table>					Highest E for zero ignition probability		Type of ignition		Confined	Unconfined	Confined	Unconfined	Bulk PETN	> 11.0	0.21	None	Deton.	PETN through 100 mesh	0.062	0.21	Deflag.	Deton.
	Highest E for zero ignition probability		Type of ignition																				
	Confined	Unconfined	Confined	Unconfined																			
Bulk PETN	> 11.0	0.21	None	Deton.																			
PETN through 100 mesh	0.062	0.21	Deflag.	Deton.																			

Fresh PETN $E_{50} = 30 \text{ mJ}^{[12]}$; aged PETN $E_{50} = 20 \text{ mJ}^{[12]}$ (artificial aging performed as isothermal @ 70 °C for 113 days in absence of air or moisture)^[12], initiation by electric spark: can be detonated by 2,000–12,000 V electric spark produced by discharging a condenser^[63], 0.036 (12,000 V, 2.6 micron, for zero ignition, 500 MMF capacitance, 0.005 in gap setting)^[133], 0.144 (24,000 V, special crystal, for zero ignition, 500 MMF capacitance, 0.005 in gap setting)^[133]

Highest energy (J) for zero ignition probability^[133]:

Results from ^[133]	Bureau of Mines, 1943	Bureau of Mines, 1946	NOL, 1959
0.036	0.31	0.062	0.085

PETN particle size effects (*U.S. standard sieve series, tested with steel phonograph needles)^[135]:

Sample particle size*	50% point energy (J)		
	1 mil foil	10 mil foil	% expl.
On 35	0.162	4.0	0
Through 35 on 42	0.150	2.42	0
Through 42 on 60	0.165	1.83	0
Through 60 on 80	0.138	1.23	0
Through 80 on 115	0.135	1.00	15
Through 115 on 325	0.098	0.408	33

Data from^[135]:

Material	50% point energy (J)		
	3 mil foil	10 mil foil	% expl.
PETN (DuPont)	0.19	0.75	8

Heated explosives^[135]:

$T(^{\circ}\text{C})$	50% energy (J)		
	3 mil foil	10 mil foil	% expl.
22	0.25	0.70	50
50	0.24	0.78	42
75	0.21	0.70	15
100	0.18	0.60	42
125	0.26	0.79	40

N [%]	17.72															
$\Omega(\text{CO}_2)$ [%]	−10.12															
$T_{\text{phase transitions}}$ [°C]	130 phase transition (2 polymorphs of PETN: tetragonal and orthorhombic) ^[20] , 130.0 PETN I (most common phase) → PETN II ^[21] , 130 tetragonal (phase-I) – orthorhombic (phase-II) ^[44] , <130 rapid transformation of orthorhombic (phase-II) – tetragonal (phase-I) ^[44] , high pressure phase transitions: phase transition ~96 GPa @ RT, irreversible under hydrostatic conditions ^[87] , high T phase transition: $P\text{-}42_1c \rightarrow Pcnb$ ^[87] , early reports stated form I stable to mpt (142.9 °C), later, observed that form II melts 0.2 °C higher than form I suggesting that at this temperature form II is the stable form ^[134] , form II forms on the face of form I growing from supercooled melt ^[134] , at $T < 130$ °C form II rapidly converts to form I ^[134]															
$T_{\text{m.p.}}$ [°C]	<p>142.9^[11, 21], 141^[13, 54, 86, 99, 102, 119, 127], 141.3^[20, 41, 75, 107, 111, 138], 143^[22, 42, 109], 142 (crystals)^[38], 140–141 (technical grade)^[38], 150 (single-crystal, thermocycle @ 2,500 °C/s, nanocalorimetric curve)^[56], 140^[58, 91, 107], 140.82 (endo, onset), 142.10 (endo, peak max.) (DSC @ 10 °C/min)^[61], 140–141^[63], 141.3 (pure)^[8, 63], 138.0–138.5 (commercial PETN)^[8, 64], 140.5–141.0 (pure PETN)^[64], 140 (endo, max., DSC)^[68], 139.45 (endo, DSC @ 10 °C/min, 1–10 mg sample, unsealed but covered Al pans)^[76], 142 (aged sample)^[91], ~145 (standard sample, DTA)^[91], 140 (standard sample)^[91], 140.1 (onset), 142.4 (peak max), 144.2 (end T) (DSC @ 10.0 K/min, pinhole cover)^[98], 141–142^[117]</p> <p>DSC (@ 10 °C/min, sealed into Al pinhole pans, 1 mg sample, Ar) mpt. vs. specific surface area (SSA) (Lötzsch air permeametry)^[90]:</p> <table><tr><td>PETN sample type</td><td>Average max. mpt. (°C)</td><td>SSA (cm² g^{−1})</td></tr><tr><td>Spherical</td><td>142.4</td><td>−5,550</td></tr><tr><td>Needle shaped</td><td>142.1</td><td>−6,750</td></tr><tr><td>Spherical with same SSA as PETN “D”</td><td>141.9</td><td>−7,200</td></tr><tr><td>PETN “D”</td><td>142.0</td><td>−7,200</td></tr></table>	PETN sample type	Average max. mpt. (°C)	SSA (cm ² g ^{−1})	Spherical	142.4	−5,550	Needle shaped	142.1	−6,750	Spherical with same SSA as PETN “D”	141.9	−7,200	PETN “D”	142.0	−7,200
PETN sample type	Average max. mpt. (°C)	SSA (cm ² g ^{−1})														
Spherical	142.4	−5,550														
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PETN “D”	142.0	−7,200														

DSC, flame sealed in glass microampoules, N ₂ @ 50 mL/min ^[109] :				
Heating rate (K/min)	<i>n</i>	Mass (mg)	Endotherm, <i>T</i> _{min} (°C)	Δ <i>H</i> _{fus} (J/g)
20	4	0.125	144	109
10	4	0.297	143	148
9	3	0.280	143	128
8	4	0.298	142	147
7	3	0.330	142	145
6	3	0.326	142	117
5	3	0.284	143	110
4	3	0.289	142	117
3	3	0.282	141	102
2	3	0.301	140	120
1	3	0.352	140	137
PETN eutectics ^[20] :				
Composition			mpt. (°C)	
1.5% PETN, 98.5% NG			12.3	
20% PETN, 80% <i>m</i> -dinitrobenzene			82.4	
10% PETN, 90% 2,4-dinitrotoluene			67.3	
13% PETN, 87% TNT			76.1	
30% PETN, 70% tetryl			111.3	
20% PETN, 80% mannitol hexanitrate			101.3	
<i>T</i> _{b.p.} [°C]	160 °C @ 2 mm Hg ^[20, 63, 64] , 180 °C @ 50 mm Hg ^[20, 63, 64] , 200 °C ± 10 @ 760 mm Hg ^[63, 64]			
<i>T</i> _{dec.} [°C]	179 (DSC @ 5 °C/min), 421 K (DTA) ^[5, 71] , 225 (@ 5 °C/s) ^[11] , 210 (@ 10 °C/s) ^[11] , 210 (exotherm peak maximum, @ 20 °C/s) ^[42] , sublimation and dec. occur concurrently ^[54] , dec. begins @ 75 (activation energy of 192 kJ mol ⁻¹ obtained between 75–130 °C) ^[54] , 170 (exotherm reaction) ^[58] , 100 (TG onset) ^[58] , 192.35 (exo, onset), 201.62 (exo, peak max) DSC @ 10 °C/min ^[61] , 165 (onset) ^[72] , 202.0 (DTA) ^[79] , 192.07 (exo, DSC @ 10 °C/min, 1–10 mg sample, unsealed but covered Al pans) ^[76] , 142.98 (endo, crude sample, peak max., DSC @ 10 °C/min, 1–10 mg sample, unsealed but covered Al pans) ^[76] , 141.30 (endo, 93.97 mol% purity, DSC @ 10 °C/min, 1–10 mg sample, unsealed but covered Al pans) ^[76] , 143.37 (endo, purified sample, peak max., DSC @ 10 °C/min, 1–10 mg sample, unsealed but covered Al pans) ^[76] , 205–215 (DSC @ 10 °C/min, sealed into Al pinhole pans, 1 mg sample, Ar) ^[90] , ~110 (<i>T</i> _{db} , dec. onset, aged sample, TGA) ^[91] , 183 (<i>T</i> _{idb} , intensive dec. onset,			

aged sample, DTA)^[91], 160–180 (T_{idb} , intensive dec. onset, standard samples, DTA)^[91], 167 (onset), 206 (exo peak max) (DSC @ 10 °C/min, sealed Al pan with pinhole lid, PETN type RPS 94–01B)^[96], 187.7 (onset), 202.9 (peak max), 216.3 (end T) (DSC @ 10.0 K/min, pinhole cover)^[98], 200 (DTA, max. mass loss @ 10 K/Min, 8–10 mg sample, open Pt pan)^[109], >210 (rapid dec. sometimes with detonation at atmospheric pressure)^[20], 140–145^[138]

@ 8 °C/min: $T_{\text{idb}} = 171.1$, $T_w = 182.3$, $T_{\text{max}} = 203.5$ ^[50]

@ 16 °C/min: $T_{\text{idb}} = 193.7$, $T_w = 206.6$, $T_{\text{max}} = 215.4$ ^[50], $T_{\text{cr}} = 200$ – 203 ^[50]

230 (exo peak max., sharp peak suggesting rapid dec., DSC)^[68]

DSC, flame sealed in glass microampoules, N_2 @ 50 mL/min^[109]:

Heating rate (K/min)	n	Mass (mg)	Exotherm, T_{min} (°C)	Exotherm, T_{max} (°C)	ΔH (J/g)
20	4	0.125	198	212	1,971
10	4	0.297	193	202	3,874
9	3	0.280	192	201	3,358
8	4	0.298	191	199	4,032
7	3	0.330	188	196	3,634
6	3	0.326	189	195	4,060
5	3	0.284	186	194	3,734
4	3	0.289	183	192	2,985
3	3	0.282	181	189	2,919
2	3	0.301	178	183	3,553
1	3	0.352	172	173	4,096

Nonisothermal TG data^[142]:

β/K min^{-1}	T_{ot}	T_i	Mass loss/%		$L_{\text{max}}/\%$ min^{-1}	$T_p/^\circ\text{C}$	$T_{\text{oe}}/^\circ\text{C}$
			Stage 1	Residue/%			
5.0	172.7	128.9	98.52	0.27	–24.70	186.9	199.9
7.0	176.3	129.1	97.34	0.93	–33.47	190.1	205.8
10.0	180.8	129.3	96.11	2.41	–48.17	194.5	214.6
15.0	186.0	129.5	95.66	3.75	–73.22	199.4	224.4

T_{ot} = onset T of dec., T_{oe} = onset T of end of dec., T_i = initial T for thermal dec.,

T_p = peak T of mass loss rate, stage 1 = from initial T to end T of DTG peak,

L_{max} = max. mass loss rate

ρ [g cm ⁻³]	<p>1.827 (@ 123 K), 1.750 (@ 298 K, gas pycnometer), 1.67 (@ 293 K)^[1], 1.772^[3], 1.778^[11], 1.77 (crystal)^[13, 77, 119], 1.778 (tetragonal crystals)^[20], 1.716 (orthorhombic crystals)^[20], 1.77 (@ TMD)^[26], 1.76 (nominal)^[26, 91], 1.76^[59], sp. gr. = 1.77 (in cryst. form)^[63], 1.773 (single crystal)^[72], 1.78 (@ TMD)^[91, 112], 1.78^[99], 1.765 (crystal)^[107], 1.74 (pressed ρ @ 40,000 psi)^[107], 1.60 (compressed)^[107], 1.7599 (pycnometer)^[109], 1.778 (X-ray)^[109], sp. gr. = 1.77^[117], 1.765^[127], 1.77^[138]</p> <p>Loading densities^[13]: 1.37 @ 3,000 psi^[13], 1.58 @ 5,000 psi^[13], 1.64 @ 10,000 psi^[13], 1.71 @ 20,000^[13], 1.72 @ 30,000 psi^[13], 1.74 @ 40,000 psi^[13]</p> <p>Loading densities: 1.48 g cm⁻³ @ 5 kpsi^[37, 119], 1.61 @ 10 kpsi^[37, 119], crystal = 1.76^[37, 119]</p> <p>Packing density as function of loading press, pressure (kg/cm²)/ρ (g cm⁻³): 351/1.575, 703/1.638, 1,406/1.710, 2,109/1.725, 2,812/1.740^[7, 20, 63]</p> <p>Crystal density^[21]:</p> <table><tr><th>Method of determination</th><th>T (°C)</th><th>Crystal form</th><th>Crystal density (g/cm³)</th></tr><tr><td>X-ray calculation</td><td>22</td><td>I</td><td>1.778</td></tr><tr><td>X-ray Calculation</td><td>136</td><td>II</td><td>1.716</td></tr><tr><td>Exptl.</td><td>22</td><td>I</td><td>1.778</td></tr></table> <p>Under compression^[21]:</p> <table><tr><th>Pressure (psi)</th><th>Density (g/cm³)</th></tr><tr><td>5,000</td><td>1.58</td></tr><tr><td>10,000</td><td>1.64</td></tr><tr><td>20,000</td><td>1.71</td></tr><tr><td>30,000</td><td>1.73</td></tr><tr><td>40,000</td><td>1.74</td></tr></table>	Method of determination	T (°C)	Crystal form	Crystal density (g/cm ³)	X-ray calculation	22	I	1.778	X-ray Calculation	136	II	1.716	Exptl.	22	I	1.778	Pressure (psi)	Density (g/cm ³)	5,000	1.58	10,000	1.64	20,000	1.71	30,000	1.73	40,000	1.74
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5,000	1.58																												
10,000	1.64																												
20,000	1.71																												
30,000	1.73																												
40,000	1.74																												
Heat of formation	-128.7 kcal mol ⁻¹ (enthalpy of form.) ^[20, 91] , -110.34 kcal mol ⁻¹ (heat of form., ΔH°_f @ 25 °C) ^[20, 21] , 390 kcal/kg (ΔH_f) ^[63] , 123 kcal/mol (ΔH_f) ^[63] , -515.3 kJ mol ⁻¹ (enthalpy of form.) ^[72] , -125.5 kcal/mol (ΔH_f) ^[77] , -538.48 kJ/mol ^[109, 112] , -128.8 kcal/mol (ΔH_f (s)) ^[59] , -401 cal/g ^[3] , 383 kcal/kg ^[13, 35] , -398 kcal/kg (enthalpy of form.) ^[74] , 379.5 kcal/kg ^[117]																												
Heat of combustion	1,960 kcal/kg ^[13, 35, 119] , $\Delta H_c = -8,140$ kJ/kg ^[58] , 1,974 kcal/kg ^[63] , 618.7 kcal/mol ^[20] , 1,962 (@ C°) ^[117] , $\Delta H^\circ_c = -618.7$ kcal/mol ^[21]																												

	Calcd. (EXPLOS 6.03)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^{\circ}$ [kJ kg ⁻¹]	5,995	165 kcal/100 g [H ₂ O (l)] (calcd.) ^[26] 151 kcal/100 g [H ₂ O (g)] (calcd.) ^[26] 1,385 kcal/kg ^[35, 117] 1.51 kcal/g (Q_{max} , calcd.) ^[59] 5,866 ^[72] 1,372 kcal/kg (@ 1.700 g cm ⁻³ , calcd.) [H ₂ O vapor] ^[74] 1,391 kcal/kg (@ 1.7650 g cm ⁻³ , calcd.) [H ₂ O vapor] ^[74] 1,416 cal/g (calcd.) ^[116] 153.7 kcal/100 g (@ 1.50 g cm ⁻³ , constant volume) [H ₂ O (l)] ^[127] 6,401.52 J/g (explosion heat) ^[138]	1,385 cal/g ^[13, 119] 1,410 kcal/kg ^[18] 6,404 ^[19] 1.65 kcal/g [H ₂ O (l)] ^[20] 1.51 kcal/g [H ₂ O (g)] ^[20] 1,490 kcal/kg [H ₂ O (l)] ^[26] 1,370 kcal/kg [H ₂ O (g)] ^[26] 1,530 kcal/kg (tests using 1 kg PETN) ^[63] 1,350 kcal/kg (@ 1.700 g cm ⁻³) [H ₂ O vapor] ^[74] 1,422 kcal/kg (@ 1.7650 g cm ⁻³) [H ₂ O vapor] ^[74] Calorimetric heat of detonation, 25 g cylinder sample, 1.2 cm diameter, detonated in isothermal calorimetry bomb under 65 Pa vacuum) ^[62] ; $\rho = 1.73$ g cm ⁻³ , 6,234 J/g (25 °C, H ₂ O (l)), 10,795 J/cm ³ , 11,096 J/cm ³ (TMD) ^[62] 6,226 J/g (@ 1.735 g cm ⁻³ , [H ₂ O (l)], heavily confined) ^[70] 5,739 J/g (@ 1.735 g cm ⁻³ , [H ₂ O (g)], heavily confined) ^[70] 6,297 J/g (@ 1.496 g cm ⁻³ , [H ₂ O (l)], heavily confined) ^[70] 5,824 J/g (@ 1.496 g cm ⁻³ , [H ₂ O (g)], heavily confined) ^[70]

			<p>6,293 J/g (@ 1.34 g cm⁻³, [H₂O (l)], heavily confined)^[70]</p> <p>5,817 J/g (@ 1.34 g cm⁻³, [H₂O (g)], heavily confined)^[70]</p> <p>5,710 J/g (@ 1.263 g cm⁻³, cylinder test)^[70]</p> <p>5,655 J/g (@ 1.503 g cm⁻³, cylinder test)^[70]</p> <p>6,130 J/g (@ 1.763 g cm⁻³, cylinder test)^[70]</p> <p>10.1 GPa (@ 1.710 g cm⁻³, detonation energy, PETN containing ~5% of organic phlegmatizer)^[78]</p> <p>2,240 cal/cm³ (voidless, volumetric heat of explosion)^[119]</p> <p>2,260 cal/cm³ (pressed @ 10,000 psi, volumetric heat of explosion)^[119]</p>
T_{ex} [K]	3,958	<p>4,500 (@ 1.67 g cm⁻³)^[28]</p> <p>3,018 (@ 1.67 g cm⁻³)^[28]</p> <p>2,340 (@ 1.67 g cm⁻³)^[28]</p> <p>4,400 (@ 1.77 g cm⁻³)^[28]</p> <p>2,833 (@ 1.77 g cm⁻³)^[28]</p> <p>2,070 (@ 1.77 g cm⁻³)^[28]</p> <p>4,850 (@ 1.00 g cm⁻³)^[28]</p> <p>3,970 (@ 1.00 g cm⁻³)^[28]</p> <p>4,300 (@ 1.00 g cm⁻³)^[28]</p> <p>5,280 (@ 1.60 g cm⁻³, calcd.)^[35]</p> <p>2,812 (@ 1.78 g cm⁻³, calcd.)^[35]</p>	<p>2,833 (@ 1.77 g cm⁻³)^[11]</p> <p>3,970 (@ 1.0 g cm⁻³)^[11]</p> <p>4,493 (@ 0.50 g cm⁻³)^[11]</p> <p>4,442 (@ 0.25 g cm⁻³)^[11]</p> <p>5,684 (@ 1.56 g cm⁻³)^[35]</p> <p>3,400 (@ 1.67 g cm⁻³)^[28]</p> <p>4,200 (single crystal)^[28]</p> <p>5,783 (@ 1.0 g cm⁻³)^[35]</p> <p>6,900 (@ 1.48 g cm⁻³)^[35]</p> <p>5,125 (@ 1.0 g cm⁻³, radiation method)^[35]</p> <p>5,700 (@ 1.2 g cm⁻³, radiation method)^[35]</p>

	<p>4,145 (@ 1.77 g cm⁻³, $\Delta H_f = -125.5$ kcal/mol, calcd., KLRR/C, THEOSTAR-T)^[77]</p> <p>4,298 (@ 1.77 g cm⁻³, $\Delta H_f = -125.5$ kcal/mol, calcd., BKWC, THEOSTAR-T)^[77]</p> <p>3,528 (@ 1.77 g cm⁻³, $\Delta H_f = -125.5$ kcal/mol, calcd., BKWR, THEOSTAR-T)^[77]</p> <p>4,001 (@ 1.778 g cm⁻³ (100% TMD), calcd. CHEETAH-6)^[93]</p> <p>3,018 (@ 1.67 g cm⁻³, $\Delta H_f^0 = -1,264$ kJ/kg, calcd., FORTRAN BKW)^[113]</p> <p>3,970 (@ 1.00 g cm⁻³, $\Delta H_f^0 = -1,264$ kJ/kg, calcd., FORTRAN BKW)^[113]</p> <p>4,345 °C (@ 1.50 g cm⁻³)^[127]</p> <p>4,230 °C^[138]</p> <p>3,330 (@ 1.76 g cm⁻³, calcd. BKWR)^[14]</p> <p>3,400 (@ 1.70 g cm⁻³, calcd. BKWR)^[14]</p> <p>3,520 (@ 1.60 g cm⁻³, calcd. BKWR)^[14]</p> <p>3,710 (@ 1.45 g cm⁻³, calcd. BKWR)^[14]</p> <p>3,940 (@ 1.23 g cm⁻³, calcd. BKWR)^[14]</p> <p>4,150 (@ 0.99 g cm⁻³, calcd. BKWR)^[14]</p> <p>4,240 (@ 0.88 g cm⁻³, calcd. BKWR)^[14]</p>	<p>6,550 (@ 1.5 g cm⁻³, radiation method)^[35]</p> <p>4,200 (@ 1.77 g cm⁻³, luminosity method)^[35]</p> <p>4,230 °C (tests using 1 kg PETN)^[63]</p> <p>4,200^[77]</p> <p>4,400 (@ 1.60 g cm⁻³)^[14]</p>
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		<p>4,460 (@ 0.48 g cm⁻³, calcd. BKWR)^[14]</p> <p>4,470 (@ 0.30 g cm⁻³, calcd. BKWR)^[14]</p> <p>4,460 (@ 0.25 g cm⁻³, calcd. BKWR)^[14]</p> <p>4,280 (@ 1.76 g cm⁻³, calcd. BKWS)^[14]</p> <p>4,320 (@ 1.70 g cm⁻³, calcd. BKWS)^[14]</p> <p>4,390 (@ 1.60 g cm⁻³, calcd. BKWS)^[14]</p> <p>4,490 (@ 1.45 g cm⁻³, calcd. BKWS)^[14]</p> <p>4,600 (@ 1.23 g cm⁻³, calcd. BKWS)^[14]</p> <p>4,640 (@ 0.99 g cm⁻³, calcd. BKWS)^[14]</p> <p>4,640 (@ 0.88 g cm⁻³, calcd. BKWS)^[14]</p> <p>4,560 (@ 0.48 g cm⁻³, calcd. BKWS)^[14]</p> <p>4,450 (@ 0.30 g cm⁻³, calcd. BKWS)^[14]</p> <p>4,400 (@ 0.25 g cm⁻³, calcd. BKWS)^[14]</p>	
p_{C-1} [kbar]	31.6	<p>226 (@ 1.60 g cm⁻³, calcd.)^[35]</p> <p>30.84 GPa (CHEETAH 2.0)^[6]</p> <p>324 (@ 1.78 g cm⁻³, calcd.)^[35]</p> <p>7 (@ 0.25 g cm⁻³, calcd. thermochem.)^[53]</p> <p>24 (@ 0.5 g cm⁻³, calcd. thermochem.)^[53]</p>	<p>300^[1]</p> <p>335 (@ 1.77 g cm⁻³)^[11]</p> <p>306 (@ 1.67 g cm⁻³)^[11]</p> <p>87 (@ 0.99 g cm⁻³)^[11]</p> <p>337 (@ 1.76 g cm⁻³)^[14]</p> <p>307 (@ 1.70 g cm⁻³)^[14]</p> <p>266 (@ 1.60 g cm⁻³)^[14]</p>

	<p>335 (@ 1.77 g cm⁻³, calcd. thermochem.)^[53]</p> <p>327 (@ 1.76 g cm⁻³, calcd.)^[59]</p> <p>30.6 GPa (@ 1.77 g cm⁻³, $\Delta H_f = -125.5$ kcal/mol, calcd., KLRR/C, THEOSTAR-T)^[77]</p> <p>31.7 GPa (@ 1.77 g cm⁻³, $\Delta H_f = -125.5$ kcal/mol, calcd., BKWC, THEOSTAR-T)^[77]</p> <p>32.9 GPa (@ 1.77 g cm⁻³, $\Delta H_f = -125.5$ kcal/mol, calcd., BKWR, THEOSTAR-T)^[77]</p> <p>307 @ 1.778 g cm⁻³ (100% TMD), calcd. CHEETAH-6)^[93]</p> <p>30.44 GPa (@ 1.7599 g cm⁻³ (pycnometry density), heat of formation = -538.48 kJ/mol, CHEETAH 6.0)^[109]</p> <p>3.717 GPa (@ 0.69 g cm⁻³ (SSED density), heat of formation = -538.48 kJ/mol, CHEETAH 6.0)^[109]</p> <p>28.0 GPa (@ 1.67 g cm⁻³, $\Delta H_f^0 = -1,264$ kJ/kg, calcd., FORTRAN BKW)^[113]</p> <p>10.1 GPa (@ 1.00 g cm⁻³, $\Delta H_f^0 = -1,264$ kJ/kg, calcd., FORTRAN BKW)^[113]</p> <p>298 (@ 1.76 g cm⁻³, calcd. BKWR)^[14]</p> <p>279 (@ 1.70 g cm⁻³, calcd. BKWR)^[14]</p> <p>251 (@ 1.60 g cm⁻³, calcd. BKWR)^[14]</p> <p>215 (@ 1.45 g cm⁻³, calcd. BKWR)^[14]</p>	<p>208 (@ 1.45 g cm⁻³)^[14]</p> <p>139 (@ 1.23 g cm⁻³)^[14]</p> <p>87 (@ 0.99 g cm⁻³)^[14]</p> <p>68 (@ 0.88 g cm⁻³)^[14]</p> <p>24 (@ 0.48 g cm⁻³)^[14]</p> <p>13 (@ 0.30 g cm⁻³)^[14]</p> <p>8 (@ 0.25 g cm⁻³)^[14]</p> <p>309 (@ 1.78 g cm⁻³)^[15]</p> <p>335 (@ 1.77 g cm⁻³)^[20]</p> <p>300 (@ 1.67 g cm⁻³)^[20, 26]</p> <p>87 (@ 0.99 g cm⁻³)^[20, 26]</p> <p>340 (@ 1.77 g cm⁻³)^[26]</p> <p>224.7 (@ 1.538 g cm⁻³)^[35]</p> <p>239.9 (@ 1.568 g cm⁻³, pressed)^[35]</p> <p>31 GPa (@ 1.67 g cm⁻³)^[21]</p> <p>340,000 atm. (@ 1.77 g cm⁻³, luminosity method)^[35]</p> <p>2.64 GPa (@ 0.50 g cm⁻³)^[52]</p> <p>31.5 GPa (@ 1.77 g cm⁻³)^[52]</p> <p>6.6 (@ 0.25 g cm⁻³)^[53]</p> <p>21.2 (@ 0.5 g cm⁻³)^[53]</p> <p>79.3 (@ 1.0 g cm⁻³)^[53]</p> <p>254.8 (@ 1.67 g cm⁻³)^[53]</p> <p>292.1 (@ 1.77 g cm⁻³)^[53]</p> <p>31.5 GPa (@ 1.763 g cm⁻³)^[70]</p>
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	<p>87 (@ 1.0 g cm⁻³, calcd. thermochem.)^[53]</p> <p>300 (@ 1.67 g cm⁻³, calcd. thermochem.)^[53]</p> <p>161 (@ 1.23 g cm⁻³, calcd. BKWR)^[14]</p> <p>104 (@ 0.99 g cm⁻³, calcd. BKWR)^[14]</p> <p>82 (@ 0.88 g cm⁻³, calcd. BKWR)^[14]</p> <p>28 (@ 0.48 g cm⁻³, calcd. BKWR)^[14]</p> <p>13 (@ 0.30 g cm⁻³, calcd. BKWR)^[14]</p> <p>10 (@ 0.25 g cm⁻³, calcd. BKWR)^[14]</p> <p>312 (@ 1.76 g cm⁻³, calcd. BKWS)^[14]</p> <p>289 (@ 1.70 g cm⁻³, calcd. BKWS)^[14]</p> <p>254 (@ 1.60 g cm⁻³, calcd. BKWS)^[14]</p> <p>208 (@ 1.45 g cm⁻³, calcd. BKWS)^[14]</p> <p>153 (@ 1.23 g cm⁻³, calcd. BKWS)^[14]</p> <p>100 (@ 0.99 g cm⁻³, calcd. BKWS)^[14]</p> <p>78 (@ 0.88 g cm⁻³, calcd. BKWS)^[14]</p> <p>26 (@ 0.48 g cm⁻³, calcd. BKWS)^[14]</p>	<p>24.0 GPa (@ 1.503 g cm⁻³)^[70]</p> <p>16.0 GPa (@ 1.263 g cm⁻³)^[70]</p> <p>31.7 GPa (@ 1.77 g cm⁻³)^[77]</p> <p>32.0 GPa (@ 1.77 g cm⁻³, cylinder test)^[78]</p> <p>30.0 GPa (@ 1.67 g cm⁻³)^[113]</p> <p>8.7 GPa (@ 1.00 g cm⁻³)^[113]</p> <p>31.5 GPa (@ 1.763 g cm⁻³)^[114]</p> <p>24.0 GPa (@ 1.503 g cm⁻³)^[114]</p> <p>16.0 GPa (@ 1.263 g cm⁻³)^[114]</p> <p>327 (voidless)^[119]</p> <p>264 (pressed @ 10,000 psi)^[119]</p> <p>0.253 Mbar^[119]</p> <p>Data from^[20]:</p> <table><tr><th>ρ (g/cm³)</th><th>Dimen- sions of PETN: diameter × length (cm); shock Elec- tric effect measure- ments</th><th>Detona- tion pressure (kbar)</th></tr><tr><td>1.764</td><td>5 × 3</td><td>338</td></tr><tr><td>1.763</td><td>2.5 × 1.3</td><td>333</td></tr><tr><td>1.763</td><td>2.5 × 2.5</td><td>340</td></tr><tr><td>1.763</td><td>5 × 1.3</td><td>338</td></tr><tr><td>1.763</td><td>5 × 2.5</td><td>340</td></tr><tr><td>1.762</td><td>5 × 2.5</td><td>339</td></tr><tr><td>1.758</td><td>2.5 × 2.5</td><td>333</td></tr><tr><td>1.71</td><td>2.5 × 2.5</td><td>309</td></tr></table>	ρ (g/cm ³)	Dimen- sions of PETN: diameter × length (cm); shock Elec- tric effect measure- ments	Detona- tion pressure (kbar)	1.764	5 × 3	338	1.763	2.5 × 1.3	333	1.763	2.5 × 2.5	340	1.763	5 × 1.3	338	1.763	5 × 2.5	340	1.762	5 × 2.5	339	1.758	2.5 × 2.5	333	1.71	2.5 × 2.5	309
ρ (g/cm ³)	Dimen- sions of PETN: diameter × length (cm); shock Elec- tric effect measure- ments	Detona- tion pressure (kbar)																											
1.764	5 × 3	338																											
1.763	2.5 × 1.3	333																											
1.763	2.5 × 2.5	340																											
1.763	5 × 1.3	338																											
1.763	5 × 2.5	340																											
1.762	5 × 2.5	339																											
1.758	2.5 × 2.5	333																											
1.71	2.5 × 2.5	309																											

		12 (@ 0.30 g cm ⁻³ , calcd. BKWS) ^[14] 9 (@ 0.25 g cm ⁻³ , calcd. BKWS) ^[14]	<table><tr><td>1.70</td><td>2.5 × 2.5</td><td>307</td></tr><tr><td>1.69</td><td>2.5 × 2.5</td><td>304</td></tr><tr><td>1.60</td><td>2.5 × 2.5</td><td>266</td></tr><tr><td>1.59</td><td>2.5 × 2.5</td><td>259</td></tr><tr><td>1.53</td><td>2.5 × 2.5</td><td>225</td></tr><tr><td>1.46</td><td>2.5 × 2.5</td><td>198</td></tr><tr><td>1.45</td><td>2.5 × 2.5</td><td>208</td></tr><tr><td>1.44</td><td>2.5 × 2.5</td><td>199</td></tr><tr><td>1.38</td><td>2.5 × 2.5</td><td>173</td></tr><tr><td>1.23</td><td>2.5 × 2.5</td><td>138</td></tr><tr><td>0.99</td><td>2.5 × 1.3</td><td>87</td></tr><tr><td>0.95</td><td>2.5 × 1.3</td><td>85</td></tr><tr><td>0.93</td><td>2.5 × 2.5</td><td>77</td></tr><tr><td>0.93</td><td>2.5 × 3.8</td><td>72</td></tr><tr><td>0.89</td><td>2.5 × 2.5</td><td>71</td></tr><tr><td>0.88</td><td>2.5 × 2.5</td><td>68</td></tr><tr><td colspan="3">Optical (smear camera) measurements</td></tr><tr><td>0.48</td><td>3.8 × 2.5</td><td>24</td></tr><tr><td>0.30</td><td>3.8 × 1.3</td><td>24</td></tr><tr><td>0.29</td><td>3.8 × 2.5</td><td>15</td></tr><tr><td>0.27</td><td>3.8 × 1.3</td><td>5</td></tr><tr><td colspan="3">Quartz crystal measurements</td></tr><tr><td>0.25</td><td>4.5 × 2.5</td><td>8</td></tr><tr><td>0.25</td><td>4.5 × 2.5</td><td>7</td></tr><tr><td>0.25</td><td>4.5 × 3.8</td><td>6</td></tr></table>	1.70	2.5 × 2.5	307	1.69	2.5 × 2.5	304	1.60	2.5 × 2.5	266	1.59	2.5 × 2.5	259	1.53	2.5 × 2.5	225	1.46	2.5 × 2.5	198	1.45	2.5 × 2.5	208	1.44	2.5 × 2.5	199	1.38	2.5 × 2.5	173	1.23	2.5 × 2.5	138	0.99	2.5 × 1.3	87	0.95	2.5 × 1.3	85	0.93	2.5 × 2.5	77	0.93	2.5 × 3.8	72	0.89	2.5 × 2.5	71	0.88	2.5 × 2.5	68	Optical (smear camera) measurements			0.48	3.8 × 2.5	24	0.30	3.8 × 1.3	24	0.29	3.8 × 2.5	15	0.27	3.8 × 1.3	5	Quartz crystal measurements			0.25	4.5 × 2.5	8	0.25	4.5 × 2.5	7	0.25	4.5 × 3.8	6
1.70	2.5 × 2.5	307																																																																												
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0.25	4.5 × 2.5	7																																																																												
0.25	4.5 × 3.8	6																																																																												
VoD [m s ⁻¹]	8,525	8,274 (@ 1.76 g cm ⁻³) (CHEETAH 2.0) ^[4] 8,280 (@ 1.77 g cm ⁻³ , calcd.) ^[26] 8,340 (@ 1.78 g cm ⁻³ , calcd.) ^[35] 8,350 (@ 1.67–1.70 g cm ⁻³ , average value from lit.) ^[33] 8,300 (@ 1.70 g cm ⁻³) ^[33]	8,000 ^[1] 8,270 (@ 1.763 g cm ⁻³) ^[70] 7,480 (@ 1.503 g cm ⁻³) ^[70] 6,590 (@ 1.263 g cm ⁻³) ^[70] 8,260 (@ 1.76 g cm ⁻³) ^[26] 8,300 (@ 1.77 g cm ⁻³) ^[7]																																																																											

	2,830 (@ 0.25 g cm ⁻³ , calcd. thermochem.) ^[53]	8,270 (@ 1.76 g cm ⁻³) ^[6, 14]
	3,800 (@ 0.5 g cm ⁻³ , calcd. thermochem.) ^[53]	8,070 (@ 1.7 g cm ⁻³) ^[6, 14]
	5,480 (@ 1.0 g cm ⁻³ , calcd. thermochem.) ^[53]	7,750 (@ 1.6 g cm ⁻³) ^[6, 14]
	7,980 (@ 1.67 g cm ⁻³ , calcd. thermochem.) ^[53]	7,180 (@ 1.45 g cm ⁻³) ^[6, 14]
	8,300 (@ 1.77 g cm ⁻³ , calcd. thermochem.) ^[53]	6,370 (@ 1.23 g cm ⁻³) ^[6, 14]
	8,650 (@ 1.76 g cm ⁻³ , calcd.) ^[59]	5,480 (@ 0.99 g cm ⁻³) ^[6, 14]
	6,945 (@ sp. gr. = 1.48) ^[63]	5,060 (@ 0.88 g cm ⁻³) ^[6, 14]
	7,200 (@ sp. gr. = 1.60) ^[63]	3,600 (@ 0.48 g cm ⁻³) ^[6, 14]
	8,000 (@ sp. gr. = 1.62) ^[63]	2,990 (@ 0.3 g cm ⁻³) ^[6, 14]
	8,340 (@ sp. gr. = 1.71) ^[63]	2,830 (@ 0.25 g cm ⁻³) ^[6, 14]
	4,200 (@ sp. gr. = 0.76) ^[63]	8,300 (@ 1.70 g cm ⁻³) ^[8, 13]
	4,400 (@ sp. gr. = 0.80) ^[63]	8,260 (@ 1.76 g cm ⁻³) ^[10]
	4,860 (@ sp. gr. = 0.84) ^[63]	8,404 (@ 1.78 g cm ⁻³) ^[15]
	5,120 (@ sp. gr. = 0.91) ^[63]	7,975 (@ 1.67 g cm ⁻³) ^[11, 21]
	5,320 (@ sp. gr. = 1.00) ^[63]	8,260 (@ 1.76 g cm ⁻³) ^[11]
	6,950 (@ sp. gr. = 1.35) ^[63]	2,810 (@ 0.241 g cm ⁻³ , unconfined rate stick) ^[20]
	7,125 (@ sp. gr. = 1.40) ^[63]	2,730 (@ 0.201 g cm ⁻³ , unconfined rate stick) ^[20]
	7,295 (@ sp. gr. = 1.45) ^[63]	2,670 (@ 0.185 g cm ⁻³ , unconfined rate stick) ^[20]
	5,550 (@ sp. gr. = 1.00) ^[63]	7,675 (@ 1.538 g cm ⁻³ , pressed) ^[35]
	8,300 (@ sp. gr. = 1.70) ^[63]	7,794 (@ 1.568 g cm ⁻³ , pressed) ^[35]
	6,060 (@ 1 g cm ⁻³ , calcd., Kamlet method) ^[27]	8,500 (@ 1.77 g cm ⁻³) ^[28]
	8,120 (@ 1.6 g cm ⁻³ , calcd., Kamlet method) ^[27]	8,350 (@ 1.73 g cm ⁻³) ^[27, 28]
		8,100 (@ 1.66 g cm ⁻³) ^[27, 28]
		7,910 (@ 1.62 g cm ⁻³) ^[27, 28]

	<p>5,360 (@ 1 g cm⁻³, calcd., Urizar method)^[27]</p> <p>7,710 (@ 1.6 g cm⁻³, calcd., Urizar method)^[27]</p> <p>8,450 (@ 1.77 g cm⁻³, $\Delta H_f = -125.5$ kcal/mol, calcd., KLRR/C, THEOSTAR-T)^[77]</p> <p>8,670 (@ 1.77 g cm⁻³, $\Delta H_f = -125.5$ kcal/mol, calcd., BKWC, THEOSTAR-T)^[77]</p> <p>8,700 (@ 1.77 g cm⁻³, $\Delta H_f = -125.5$ kcal/mol, calcd., BKWR, THEOSTAR-T)^[77]</p> <p>8,260 (@ 1.76 g cm⁻³)^[91]</p> <p>8,710 (@ 1.630 g cm⁻³, calcd., K-J)^[98]</p> <p>8,150 (@ 1.50 g cm⁻³, calcd. K-W eqn.)^[105]</p> <p>8,481 (@ 1.7599 g cm⁻³ (pycnometry density), heat of formation = -538.48 kJ/mol, CHEETAH 6.0)^[109]</p> <p>4,293 (@ 0.69 g cm⁻³ (SED density), heat of formation = -538.48 kJ/mol, CHEETAH 6.0)^[109]</p> <p>8,056 (@ 1.67 g cm⁻³, $\Delta H_f^0 = -1,264$ kJ/kg, calcd., FORTRAN BKW)^[113]</p> <p>5,947 (@ 1.00 g cm⁻³, $\Delta H_f^0 = -1,264$ kJ/kg, calcd., FORTRAN BKW)^[113]</p> <p>8,230 (@ 1.76 g cm⁻³, calcd. BKWR)^[14]</p>	<p>7,920 (@ 1.60 g cm⁻³)^[28]</p> <p>7,420 (@ 1.51 g cm⁻³)^[27, 28]</p> <p>7,130 (@ 1.40 g cm⁻³)^[28]</p> <p>2,050 (@ 0.99 g cm⁻³, low conc. PETN deposited on polystyrene)^[28]</p> <p>8,500 (@ 1.77 g cm⁻³, luminosity method)^[35]</p> <p>8,409 (calcd. based on 1,700 g bomb sand test)^[33]</p> <p>8,142 (@ 1.72 g cm⁻³)^[39]</p> <p>8,260 (@ 1.76 g cm⁻³)^[51]</p> <p>3,600 (@ 0.50 g cm⁻³)^[52]</p> <p>7,770 (@ 1.60 g cm⁻³)^[52]</p> <p>8,220 (@ 1.77 g cm⁻³)^[52]</p> <p>3,370 (@ 0.50 g cm⁻³)^[52]</p> <p>8,060 (@ 1.77 g cm⁻³)^[27, 52]</p> <p>3,468 (@ 0.25 g cm⁻³)^[53]</p> <p>4,178 (@ 0.5 g cm⁻³)^[53]</p> <p>5,720 (@ 1.0 g cm⁻³)^[53]</p> <p>7,795 (@ 1.67 g cm⁻³)^[53]</p> <p>8,125 (@ 1.77 g cm⁻³)^[53]</p> <p>5,330 (@ sp. gr. = 0.85, iron pipe, 25 mm diameter)^[63]</p> <p>7,550 (@ sp. gr. = 1.75, Cu pipe, 15/17 mm diameter)^[63]</p> <p>3,150 (@ sp. gr. = 0.45, bakelite pipe, 6/8.5 mm diameter)^[63]</p>
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	8,020 (@ 1.70 g cm ⁻³ , calcd. BKWR) ^[14]	5,300 (@ sp. gr. = 0.91, bakelite pipe, 4.5/6.3 mm diameter) ^[63]
	7,700 (@ 1.60 g cm ⁻³ , calcd. BKWR) ^[14]	5,730 (@ sp. gr. = 1.04, bakelite pipe, 4.5/6.3 mm diameter) ^[63]
	7,270 (@ 1.45 g cm ⁻³ , calcd. BKWR) ^[14]	7,375 (@ sp. gr. = 1.45, bakelite pipe, 4.5/6.3 mm diameter) ^[63]
	6,710 (@ 1.23 g cm ⁻³ , calcd. BKWR) ^[14]	8,500 (@ sp. gr. = 1.72, bakelite pipe, 4.5/6.3 mm diameter) ^[63]
	6,010 (@ 0.99 g cm ⁻³ , calcd. BKWR) ^[14]	3,965 (@ sp. gr. = 0.50, Cu pipe, 15/17 mm diameter) ^[63]
	5,650 (@ 0.88 g cm ⁻³ , calcd. BKWR) ^[14]	5,615 (@ sp. gr. = 1.03, glass pipe, 11.4/13 mm diameter) ^[63]
	4,240 (@ 0.48 g cm ⁻³ , calcd. BKWR) ^[14]	6,355 (@ sp. gr. = 1.22, Cu tube, 10/10.6 mm diameter) ^[63]
	3,570 (@ 0.30 g cm ⁻³ , calcd. BKWR) ^[14]	7,420 (@ sp. gr. = 1.50, without confinement) ^[63]
	3,380 (@ 0.25 g cm ⁻³ , calcd. BKWR) ^[14]	7,913 (@ sp. gr. = 1.62, without confinement) ^[63]
	8,670 (@ 1.76 g cm ⁻³ , calcd. BKWS) ^[14]	8,350 (@ sp. gr. = 1.73, without confinement) ^[63]
	8,430 (@ 1.70 g cm ⁻³ , calcd. BKWS) ^[14]	8,340 (@ 1.712 g cm ⁻³ , Dautriche method, Cu tube, 10 mm diameter, compressed under 2,500 kg/cm ²) ^[64]
	8,030 (@ 1.60 g cm ⁻³ , calcd. BKWS) ^[14]	5,330 (@ 0.85 g cm ⁻³ , slightly compressed material, iron pipe, 25 mm internal diameter) ^[64]
	7,480 (@ 1.45 g cm ⁻³ , calcd. BKWS) ^[14]	
	6,760 (@ 1.23 g cm ⁻³ , calcd. BKWS) ^[14]	8,000 (@ 1.62 g cm ⁻³ , PETN compressed, <i>Kast</i>) ^[64]
	5,990 (@ 0.99 g cm ⁻³ , calcd. BKWS) ^[14]	5,520 (@ 1 g cm ⁻³) ^[27]
	5,610 (@ 0.88 g cm ⁻³ , calcd. BKWS) ^[14]	7,740 (@ 1.6 g cm ⁻³) ^[27]
		7,980 (@ 1.67 g cm ⁻³) ^[27]

		4,120 (@ 0.48 g cm ⁻³ , calcd. BKWS) ^[14] 3,440 (@ 0.30 g cm ⁻³ , calcd. BKWS) ^[14] 3,250 (@ 0.25 g cm ⁻³ , calcd. BKWS) ^[14]	7,920 (@ 1.65 g cm ⁻³) ^[27] 6,970 (@ 1.37 g cm ⁻³) ^[27] 5,620 (@ 1.03 g cm ⁻³) ^[27] 5,330 (@ 0.97 g cm ⁻³) ^[27] 5,300 (@ 0.95 g cm ⁻³) ^[27] 8,300 (@ 1.77 g cm ⁻³) ^[77] 8,300 (@ 1.77 g cm ⁻³ , cylinder test) ^[78] 8,080 (@ 1.710 g cm ⁻³ , PETN containing ~5% of organic phlegmatizer) ^[78] 26,000 ft/s (@ 1.6 g/mL) ^[102] 7,600 (@ 1.50 g cm ⁻³) ^[105] 7,300 (@ 1.70 g cm ⁻³ (pressed p)) ^[107] 8,400 (Dautriche method) ^[107] 7,980 (@ 1.67 g cm ⁻³) ^[113] 5,480 (@ 1.00 g cm ⁻³) ^[113] 8,270 (@ 1.763 g cm ⁻³) ^[114] 7,480 (@ 1.503 g cm ⁻³) ^[114] 6,590 (@ 1.263 g cm ⁻³) ^[114] 8,300 (@ 1.70 g cm ⁻³) ^[8] 8,300 (@ 1.56 g cm ⁻³) ^[127]
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			<p>Detonation velocity vs. density; * = unconfined rate stick, † = cylinder test^[20].</p> <table> <tr> <th>ρ (g/cc)</th><th>Detonation velocity (m/s)</th><th>ρ (g/cc)</th><th>Detonation velocity (m/s)</th></tr> <tr> <td>1.773</td><td>8,300*</td><td>1.27</td><td>6,660[†]</td></tr> <tr> <td>1.765</td><td>8,280[†]</td><td>1.26</td><td>6,760[†]</td></tr> <tr> <td>1.765</td><td>8,240*</td><td>1.09</td><td>5,830[†]</td></tr> <tr> <td>1.763</td><td>8,270*</td><td>0.55</td><td>3,850*</td></tr> <tr> <td>1.762</td><td>8,250*</td><td>0.436</td><td>3,400*</td></tr> <tr> <td>1.762</td><td>8,260*</td><td>0.241</td><td>2,810*</td></tr> <tr> <td>1.51</td><td>7,440[†]</td><td>0.201</td><td>2,730*</td></tr> <tr> <td>1.51</td><td>7,490[†]</td><td>0.185</td><td>2,670*</td></tr> </table>	ρ (g/cc)	Detonation velocity (m/s)	ρ (g/cc)	Detonation velocity (m/s)	1.773	8,300*	1.27	6,660 [†]	1.765	8,280 [†]	1.26	6,760 [†]	1.765	8,240*	1.09	5,830 [†]	1.763	8,270*	0.55	3,850*	1.762	8,250*	0.436	3,400*	1.762	8,260*	0.241	2,810*	1.51	7,440 [†]	0.201	2,730*	1.51	7,490 [†]	0.185	2,670*
ρ (g/cc)	Detonation velocity (m/s)	ρ (g/cc)	Detonation velocity (m/s)																																				
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V_0 [L kg ⁻¹]	746	<p>790^[117]</p> <p>78.0 L/100 g (@ 1.50 g cm⁻³, @ STP)^[127]</p> <p>768^[138]</p>	<p>790^[13, 119]</p> <p>780^[16]</p> <p>823^[19]</p> <p>828 (@ 0 °C & 760 mm Hg)^[34]</p> <p>550 [H₂O (l)] (determined using Dolger's bomb, PETN $\rho = 1.65$ g cm⁻³)^[35, 36]</p> <p>790 [H₂O (g)] (determined using Dolger's bomb, PETN $\rho = 1.65$ g cm⁻³)^[36, 37]</p> <p>768.0 (tests using 1 kg PETN)^[63]</p>																																				

Critical diameter [cm]

Critical detonation diameter d_{c0} [mm] and SSA, S_g [cm² g⁻¹]^[72]:

S_g (cm ² g ⁻¹)	d_{c0} (mm)	S_g (cm ² g ⁻¹)	d_{c0} (mm)
Monodisperse TEN (fractions)		Polydisperse TEN	
140 (500–600 μm)	3.38	4,700	0.12
170 (400–500 μm)	3.18	7,700	0.10
340 (200–250 μm)	2.29	10,000	0.09
430 (90–160 μm)	1.73		
980 (0–90 μm)	0.86		

Critical detonation diameter d_{c0} [mm] and SSA, S_g [cm² g⁻¹] @ rel. high density (0.98–0.995) g cm⁻³^[72]:

S_g (cm ² g ⁻¹)	d_{c0} (mm)	S_g (cm ² g ⁻¹)	d_{c0} (mm)
650	1.00	2,900	0.25
1,500	0.50	8,000	0.10

d_{c0} (mm) @ mean crystal size (μm)^[72]: 0.08 @ 3, 0.20 @ 10, 0.40 @ 20^[72]

Measurements of d_c and initiation pressure (P_i)^[110]:

Form	ρ_0 (g/cc)	P_i (kbar)	d_c (mm)
single crystal	1.77	–112	8.5 < d_c < 19

0.9 mm @ 1.0 g cm⁻³, 0.025–0.1 mm particle size^[20], critical diameter, d_c decreases as charge density increases^[20]

	Data from ^[126] : <table><tr><td>Particle size (μ)</td><td>ρ₀ (g/cc)</td><td>Approx. d_c (mm)</td></tr><tr><td>1–10</td><td>1–68</td><td>0.18–0.19</td></tr></table> 3 mm (@ 1 g cm ⁻³) ^[138]	Particle size (μ)	ρ ₀ (g/cc)	Approx. d _c (mm)	1–10	1–68	0.18–0.19
Particle size (μ)	ρ ₀ (g/cc)	Approx. d _c (mm)					
1–10	1–68	0.18–0.19					
Critical T [°C]	200–203 (exptl.) ^[88, 101] , 196 (calcd.) ^[88, 101] , 192 (T _m) ^[21]						
Critical pressure [GPa]	P _{cr} = 0.48 ± 0.01 (by impact of CL-20) ^[81] , σ _{ult} = 60 MPa (by impact of CL-20) ^[81] , P _{ult} = 0.93 ± 0.03 GPa ^[81] , P _{cr} = 0.50 ± 0.02 (impact) ^[80] , P _{cr} = 0.93 ± 0.03 (DT) ^[80] , critical initiation pressure = 0.93 ± 0.03 GPa ^[131]						
Trauzl test [cm ³ , % TNT]	173% TNT ^[8, 13] , 161–189% TNT ^[20] , 173% TNT ^[28] , 161–181% TNT ^[33] , 500 cm ³ (sand tamping, 10 g sample) ^[63, 64] , 560 cm ³ (H ₂ O tamping, 10 g sample) ^[63, 64] , ~93% NG or 170% PA ^[63] , 378 cc (net expansion, <i>Brün</i>) ^[64] , 521 mL (10 g sample) ^[68] , 500 mL ^[117, 129] , 480 ^[129] , 490 ^[129] , 515 ^[129] , 520 ^[129] , 523 ^[129] , 500 cm ³ (sand tamping) ^[138] , 560 cm ³ (H ₂ O tamping) ^[138]						
Lead block compression test	130–137% TNT ^[20] , 14–16 mm (lead column, 25 g PETN) ^[138]						
Sand test [g]	62.7 g (200 g bomb) ^[8, 13] , 129–141% TNT ^[20, 33] , 57.9 g sand crushed (1,700 g bomb, 0.4 g PETN) ^[33]						
Brisance from Cu cylinder crusher method	128% PA ^[107]						
Ballistic mortar test	145% TNT ^[8, 13, 28] , 137–145% TNT ^[20, 33] , 100% (10 g sample, Al foil used as wrapper) ^[68] , 108% PA ^[107]						
Initiation efficiency	0.17 g MF minimum detonating charge ^[13] , 0.03 g LA minimum detonating charge ^[13, 119] , PETN with 35% water present can be detonated by a No. 6 blasting cap ^[20] Minimum initiating quantity of different donor charges to PETN (crystalline PETN = acceptor charge, accelerating distance = 2 mm, witness plate = lead plate); donor charge/minimum initiating quantity (mg) ^[57] : LP/20, LTNR/20, LA/10, Fine PETN/40, ultrafine RDX/10 ^[57] Very high sensitivity to initiation by explosion ^[63] , detonated by 0.01 g LA ^[63, 64]						

	<p>Minimum charges of primary explosives necessary to initiate explosion of PETN (0.4 g PETN tamped down or pressed loosely into Cu capsules of 6.2 mm inside diameter and primary charge pressed down loosely on top; or 0.4 g PETN compressed @ 2,000 kg/cm², primary charge pressed loosely on compressed PETN or pressed on top of the already pressed PETN with 500 kg/cm², 1,000 kg/cm² or 1,500 kg/cm² pressure)^[64]:</p> <table><tr><td>Pressure on PETN (kg/cm²)</td><td>0</td><td>2,000</td><td>2,000</td><td>2,000</td><td>2,000</td></tr><tr><td>Pressure on initiator (kg/cm²)</td><td>0</td><td>0</td><td>500</td><td>1,000</td><td>1,500</td></tr><tr><td>Primary explosive</td><td colspan="5">Minimum initiating charge (g)</td></tr><tr><td>Tetracene</td><td>0.16</td><td>0.250</td><td colspan="3">Dead pressed</td></tr><tr><td>MF (gray)</td><td>0.30</td><td>0.330</td><td colspan="3">Dead pressed</td></tr><tr><td>MF (white)</td><td>0.30</td><td>0.340</td><td colspan="3">Dead pressed</td></tr><tr><td>LS</td><td>0.55</td><td colspan="4">No detonation with 1 g</td></tr><tr><td>LA (technical)</td><td>0.04</td><td>0.170</td><td>0.05</td><td>0.05</td><td>0.04</td></tr><tr><td>LA (pure)</td><td>0.015</td><td>0.100</td><td>0.01</td><td>0.01</td><td>0.01</td></tr><tr><td>Silver azide</td><td>0.005</td><td>0.110</td><td>0.005</td><td>0.005</td><td>0.005</td></tr></table> <p>Limiting weight of detonation = 0.17 g MF^[117], 0.03 g LA^[117], PETN with 40% water can be detonated with No. 8 detonator^[138]</p>	Pressure on PETN (kg/cm ²)	0	2,000	2,000	2,000	2,000	Pressure on initiator (kg/cm ²)	0	0	500	1,000	1,500	Primary explosive	Minimum initiating charge (g)					Tetracene	0.16	0.250	Dead pressed			MF (gray)	0.30	0.330	Dead pressed			MF (white)	0.30	0.340	Dead pressed			LS	0.55	No detonation with 1 g				LA (technical)	0.04	0.170	0.05	0.05	0.04	LA (pure)	0.015	0.100	0.01	0.01	0.01	Silver azide	0.005	0.110	0.005	0.005	0.005
Pressure on PETN (kg/cm ²)	0	2,000	2,000	2,000	2,000																																																								
Pressure on initiator (kg/cm ²)	0	0	500	1,000	1,500																																																								
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LS	0.55	No detonation with 1 g																																																											
LA (technical)	0.04	0.170	0.05	0.05	0.04																																																								
LA (pure)	0.015	0.100	0.01	0.01	0.01																																																								
Silver azide	0.005	0.110	0.005	0.005	0.005																																																								
Gap test	Gap test = 3.9 kbar, charge ρ = 1.62 g cm ⁻³ ^[39]																																																												
LSGT [cm]	60 mm (LANL) ^[60] , ρ = 0.81 g cm ⁻³ (raw), percent voids = 54.2%, sensitivity = 69.4 mm (LANL LSGT) ^[20]																																																												
SSGT [cm]	<p>G_{50} = 5.21 mm (@ 1.757 g cm⁻³)^[21], 9.8 mm (NOL)^[60], 5.5 mm (LANL)^[60], P_{90} = 7.47 kbar (P_{90} = pressure to 90% of TMD, NSW small-scale gap test)^[73]</p> <p>LANL SSGT, ρ = 0.95 g cm⁻³, approx. brass thickness (in) vs. approx. specific surface (cm² g⁻¹) for ball-milled and precipitated PETN samples^[89]:</p>																																																												

Precipitated sample		Ball-milled sample	
Brass thickness (in)	Specific surface (cm ² g ⁻¹)	Brass thickness (inches)	Specific surface (cm ² g ⁻¹)
0.240	15,200	0.240	15,200
0.270	9,000	0.260	11,500
0.280	6,500	0.270	12,000
0.285	7,500	0.270	9,500
0.310	3,000	0.275	8,000
0.320	2,500	0.325	4,000

Gap test results from^[20]:

	Density (g/cc)	% voids	Sensitivity (mm)
NSWC SSGT	1.775	0.3	6.03
	1.576	11.5	14.38
	1.355	27.9	13.56
LANL SSGT	1.757 (pressed)	0.7	5.21

(1) = no mixed response zone, TMD = 1.78 g cm⁻³, data from^[125]:

Loading pressure (kpsi)	Density (g/cm ³)		% TMD	Sensitivity (DBG)			
	Avg.	s		Avg.	g	s _m	N
4	1.355	0.0053	76.1	2.726	0.0206	0.0215	18
8	1.440	0.0049	80.9	2.476	0.0939	0.0555	18
16	1.576	0.0058	88.5	2.621	0.0101	0.0106	18
32	1.681	0.0041	94.4	3.238	—	—	18 (1)

PETN (IS 50% point = 14 cm, type 12 tool, 2.5 kg mass, sandpaper, commercial sample, dried prior to test), TMD = 1.78 g cm⁻³^[125]:

	<table><tr><th rowspan="2">Loading pressure (kpsi)</th><th colspan="2">Density (g/cm³)</th><th rowspan="2">% TMD</th><th colspan="4">Sensitivity (DBG)</th></tr><tr><th>Avg.</th><th>s</th><th>Avg.</th><th>g</th><th>s_m</th><th>N</th></tr><tr><td>8</td><td>1.499</td><td>0.0065</td><td>84.2</td><td>1.725</td><td>0.5416</td><td>0.2529</td><td>22</td></tr><tr><td>16</td><td>1.600</td><td>0.0058</td><td>89.9</td><td>2.468</td><td>0.0459</td><td>0.2568</td><td>23</td></tr><tr><td>32</td><td>1.708</td><td>0.0047</td><td>96.0</td><td>3.555</td><td>0.0918</td><td>0.0445</td><td>23</td></tr><tr><td>64</td><td>1.775</td><td>0.0057</td><td>99.7</td><td>4.998</td><td>0.0158</td><td>0.0167</td><td>23</td></tr></table>	Loading pressure (kpsi)	Density (g/cm ³)		% TMD	Sensitivity (DBG)				Avg.	s	Avg.	g	s _m	N	8	1.499	0.0065	84.2	1.725	0.5416	0.2529	22	16	1.600	0.0058	89.9	2.468	0.0459	0.2568	23	32	1.708	0.0047	96.0	3.555	0.0918	0.0445	23	64	1.775	0.0057	99.7	4.998	0.0158	0.0167	23
Loading pressure (kpsi)	Density (g/cm ³)		% TMD	Sensitivity (DBG)																																											
	Avg.	s		Avg.	g	s _m	N																																								
8	1.499	0.0065	84.2	1.725	0.5416	0.2529	22																																								
16	1.600	0.0058	89.9	2.468	0.0459	0.2568	23																																								
32	1.708	0.0047	96.0	3.555	0.0918	0.0445	23																																								
64	1.775	0.0057	99.7	4.998	0.0158	0.0167	23																																								
	2.62 DBg @ 1.576 g cm ⁻³ (110 MPa) ^[130]																																														
5 s explosion <i>T</i> [°C]	222 ^[8] , 225 ^[8, 107] , 227 ^[8] , 228 ^[8] , 225 (dec.) ^[13, 119] , 210–220 ^[35] , 225 (dec., cook-off) ^[119] , 237 (Wood's metal bath, 40 mg) ^[130]																																														
1 s explosion <i>T</i> [°C]	255 ^[8] , 270 ^[8] , 276 ^[8] , 244 ^[13, 119]																																														
Explosion <i>T</i> [°C]	272 (0.1 s, no cap used) ^[13] , 211 (10 s) ^[13, 119] , 215 ^[20] , 202 (DTA/TG @ 6 °C/min) ^[39] , explodes violently above its mpt. @ 205–225 ^[63] , 205 ^[107] , 272 (0.1 s) ^[119]																																														
5 s ignition <i>T</i> [°C]	225 (dec., USA value) ^[35] , 205–225 (dec., Russian) ^[35] , 222 ^[84]																																														
Ignition <i>T</i> [°C]	Inflames spontaneously @ 210 ^[64] , 215 ^[64] , 205 ^[67] , 150 (calorimetric measurement) ^[84] , 205–215 ^[84]																																														
Ignition <i>T</i> (30 s delay) [°C]	202 (before storage) ^[91] , 204 (after 22 years storage in multilayered paper bags) ^[91]																																														
Detonating <i>T</i> [°C]	Explosion time vs. <i>T</i> (°C) ^[101] : <table><tr><th><i>T</i> (°C)</th><th>Explosion time (s)</th><th><i>T</i> (°C)</th><th>Explosion time (sec)</th></tr><tr><td>350</td><td>0.050</td><td>244</td><td>1.57</td></tr><tr><td>324</td><td>0.091</td><td>229</td><td>2.93</td></tr><tr><td>272</td><td>0.475</td><td>220</td><td>4.55</td></tr><tr><td>256</td><td>1.03</td><td>215</td><td>No explosion</td></tr></table>	<i>T</i> (°C)	Explosion time (s)	<i>T</i> (°C)	Explosion time (sec)	350	0.050	244	1.57	324	0.091	229	2.93	272	0.475	220	4.55	256	1.03	215	No explosion																										
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Thermal ignition <i>T</i> [°C]	175 ^[102] , 225 (5 s) ^[8] , 215 ^[117] , 202–205 ^[138] , 215 ^[119]																																														
100 °C heat test [% mass loss]	0.1% mass loss in first 48 h ^[13] , 0.0% mass loss in second 48 h ^[13] , no explosion in 100 h ^[13]																																														
75 °C int. heat test	0.02% mass loss in 48 h ^[13]																																														
LLNL reactivity test	0.10–0.14 cm ³ gas evolved per 0.25 g sample ^[20, 26]																																														

Thermal stability	<p>No significant deterioration on heating @ 100 °C for 100 h^[20], storage @ 65 °C for 20 months does not cause dec. and only slightly acidic after 24 months^[20], extremely stable when no acid is present^[8], no dec. observed after storage @ 100 °C for prolonged periods of time^[8]</p> <p>Moles gas formed per mole PETN/no. h^[42]: @ 120 °C; 0/22, 0/72^[42], @ 220 °C; 5.04/22, 5.19/72^[42], @ 320 °C; 6.32/22, 6.3/72^[42],</p> <p>7.87% (TG @ 120 °C, 48 h)^[79], red fumes form within 30 min @ $T \geq 140.5$ °C^[64]</p> <p>Nonisothermal TG data, $\beta =$ °C/min, T_{ei} = onset T of TG peaks, T_p = peak T, T_{oe} = endset T of TG peaks, T_b = critical T for thermal dec.^[98]:</p> <table><tr><th>β (°C/min)</th><th>T_{ei} (°C)</th><th>T_p (°C)</th><th>T_{oe} (°C)</th><th>T_b (°C)</th></tr><tr><td>5.0</td><td>172.7</td><td>186.9</td><td>199.9</td><td>171.2</td></tr><tr><td>7.0</td><td>176.3</td><td>190.1</td><td>205.8</td><td></td></tr><tr><td>10.0</td><td>180.8</td><td>194.5</td><td>214.6</td><td></td></tr><tr><td>15.0</td><td>186.0</td><td>199.4</td><td>224.4</td><td></td></tr></table> <p>storage @ 65 °C for 20 months does not cause instability^[107], uncrystallized and unwashed PETN is of low stability due to several impurities being present and mainly due to the acid it contains^[117], 0.1% weight loss in 40 h @ 100 °C (military PETN)^[138]</p>	β (°C/min)	T_{ei} (°C)	T_p (°C)	T_{oe} (°C)	T_b (°C)	5.0	172.7	186.9	199.9	171.2	7.0	176.3	190.1	205.8		10.0	180.8	194.5	214.6		15.0	186.0	199.4	224.4	
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Vacuum stability test [cm ³ /h]	<p>0.5 cc/40 h @ 100 °C^[13, 119], 11 + cc/40 h @ 120 °C^[13, 119], 0.2–0.5 mL/g gas evolved after 48 h @ 100 °C^[21], no significant dec.@ 100 °C for 100 h^[20], fresh PETN: $v = 0.79$ mL/g (40 h, 120 °C)^[48], aged PETN: $v = 0.22$ mL/g (40 h, 120 °C)^[48], 25.0 mL/5 g (@ 120 °C, 48 h)^[79], dec. liberates nitrogen oxides @ 140–145 °C and does so significantly within 30 minutes^[117], intense liberation of brown fumes @ 175 °C^[117], detonation @ 215 °C^[117], 0.5 cc/40 h @ 100 °C (military PETN)^[138]</p> <p>(PETN does not detonate or burn in vacuum^[64])</p>																									
Vapor pressure [atm @ °C]	<p>8×10^{-5} mm Hg @ 100 °C^[26], 5.21×10^{-6} Pa @ 25 °C^[109], 5.38×10^{-9} mm Hg @ 25 °C^[111]</p> <p>$\log_{10}P$ (mm Hg) = $14.44 - 6,352/T$ (K) for $323 < T < 371$ K^[21], $\log_{10}P$ (mm Hg) = $17.73 - 7750/T$ (K) for $383 < T < 412$ K^[21], 5.01×10^{-5} Torr @ 66 °C^[47], 18 ppt (i.e., 0.018 ppb, v/v) @ 25 °C^[49], 5.38×10^{-9} Torr @ 25 °C^[99], 0.026 ppb_v (equilibrium vapor pressure @ 300 K)^[106], 2.8×10^4 ppb_v (equilibrium vapor pressure @ 400 K)^[106]</p>																									

	<table><tr><td>Vapor pressure (cm Hg)^[63]</td><td>T (°C)</td></tr><tr><td>8.38 × 10⁻⁵</td><td>97.0</td></tr><tr><td>3.12 × 10⁻⁴</td><td>110.6</td></tr><tr><td>1.09 × 10⁻³</td><td>121.0</td></tr><tr><td>3.76 × 10⁻³</td><td>131.6</td></tr><tr><td>7.08 × 10⁻³</td><td>138.8</td></tr></table> <p>log₁₀ P(mm Hg) = 14.44–6,352/T (K) for 323< T<371 K^[21], log₁₀ P(mm Hg) = 17.73–7,750/T (K) for 383< T<412 K^[21]</p>	Vapor pressure (cm Hg) ^[63]	T (°C)	8.38 × 10 ⁻⁵	97.0	3.12 × 10 ⁻⁴	110.6	1.09 × 10 ⁻³	121.0	3.76 × 10 ⁻³	131.6	7.08 × 10 ⁻³	138.8																																				
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Evaporation T [°C]	~300 (nanocalorimetric curve, thermocycle @ 2,500 °C/s) ^[56]																																																
Burn rate [mm/s]	<p>Does not burn in tubes ≤18 mm diameter^[63], burning induced by preheating to 95 °C (linear rate of 0.047 cm/s)^[63], burns quietly when ignited (in small quantities)^[117], in tubes with 18 mm diameter can only be ignited if warmed to 95 °C and its burning rate is very low^[138], thin layer can be ignited in air and burnt smoothly^[138], 0.047 cm/s^[138], burning with constant speed can be achieved by increasing the pressure^[138]</p> <p>Relationship between burning rate and pressure: $U = 0.02 + 0.018P^{[138]}$</p> <p>Perspex tube assembly, throat diameter = 4.3 mm, gauze support, 6 mm bore diameter of Perspex tube, measured using blank nozzle with sealed lower end, standard deviation of the mean in parenthesis^[118]:</p> <table><tr><td>Explosive</td><td>Loading density (g/cm³)</td><td>Pressure (atm)</td><td>Apparent mass burning rate (g cm⁻² s⁻¹)</td></tr><tr><td>PETN 500–853 μ</td><td>0.928</td><td>27.2</td><td>0.544 (0.011)</td></tr><tr><td>PETN 500–853 μ</td><td>0.918</td><td>27.2</td><td>0.531 (0.006)</td></tr><tr><td>PETN 500–853 μ</td><td>0.936</td><td>31.6</td><td>8.86 (0.17)</td></tr><tr><td>PETN 500–853 μ</td><td>0.912</td><td>36.7</td><td>13.9 (0.53)</td></tr><tr><td>PETN 500–853 μ</td><td>0.939</td><td>52.0</td><td>47.7 (0.56)</td></tr><tr><td>PETN 500–853 μ</td><td>0.917</td><td>52.0</td><td>59.0 (0.70)</td></tr></table> <p>Mass burning rate data from^[124]:</p> <table><tr><td colspan="5">m (gm cm⁻² sec⁻¹)</td></tr><tr><td>40 atm</td><td>100 atm</td><td>200 atm</td><td>400 atm</td><td>1,000 atm</td></tr><tr><td>0.77</td><td>1.93</td><td>3.86</td><td>7.72</td><td>18</td></tr><tr><td>0.80</td><td>1.95</td><td></td><td></td><td></td></tr></table>	Explosive	Loading density (g/cm ³)	Pressure (atm)	Apparent mass burning rate (g cm ⁻² s ⁻¹)	PETN 500–853 μ	0.928	27.2	0.544 (0.011)	PETN 500–853 μ	0.918	27.2	0.531 (0.006)	PETN 500–853 μ	0.936	31.6	8.86 (0.17)	PETN 500–853 μ	0.912	36.7	13.9 (0.53)	PETN 500–853 μ	0.939	52.0	47.7 (0.56)	PETN 500–853 μ	0.917	52.0	59.0 (0.70)	m (gm cm ⁻² sec ⁻¹)					40 atm	100 atm	200 atm	400 atm	1,000 atm	0.77	1.93	3.86	7.72	18	0.80	1.95			
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	<p>Burn rate and equilibrium combustion temperature^[124]: $T_e = 3,880 \text{ K}^{[124]}$, $m = 1.93 \text{ g cm}^{-2} \text{ s}^{-1} (100 \text{ atm})^{[124]}$</p> <p>Dependence of burning rate of volatile explosives on pressure, PETN, $\rho_{\max} = 1.77 \text{ g/cm}^3^{[124]}$:</p> <table><tr><th rowspan="2">$\delta = \rho/\rho_{\max}$</th><th colspan="3">Coefficients in formulae $m (\text{g cm}^{-2} \text{ sec}^{-1}) = a + b p_{\text{atm}}^v$</th><th rowspan="2">Pressure, atm.</th></tr><tr><th>a</th><th>b</th><th>v</th></tr><tr><td>~1.0</td><td>–</td><td>0.0193</td><td>1.0</td><td>15–750</td></tr><tr><td rowspan="2">0.98</td><td>–</td><td>0.028</td><td>0.96</td><td>16–100</td></tr><tr><td>–</td><td>0.0173</td><td>1.0</td><td>500–1,500</td></tr></table> <p>Dependence of mass burning rate of volatile explosives on the relative density of the charge, PETN^[124]:</p> <table><tr><th>Initial size of particle of explosive</th><th>p, atm.</th><th colspan="6">$m (\delta)$</th></tr><tr><td rowspan="2">~5 μ</td><td rowspan="2">52</td><td>δ</td><td>0.50</td><td>0.51</td><td>0.66</td><td>0.73</td><td>0.88</td></tr><tr><td>$m (\text{g cm}^{-2} \text{ s}^{-1})$</td><td>0.99</td><td>0.85</td><td>0.86</td><td>0.88</td><td>0.99</td></tr><tr><td rowspan="2">100–400 μ</td><td rowspan="2">52</td><td>δ</td><td>0.60</td><td>0.82</td><td>0.86</td><td>0.90</td><td>–</td></tr><tr><td>$m (\text{g cm}^{-2} \text{ s}^{-1})$</td><td>0.99</td><td>1.00</td><td>0.87</td><td>0.99</td><td>–</td></tr></table> <p>PETN does not detonate or burn in vacuum^[64]</p>	$\delta = \rho/\rho_{\max}$	Coefficients in formulae $m (\text{g cm}^{-2} \text{ sec}^{-1}) = a + b p_{\text{atm}}^v$			Pressure, atm.	a	b	v	~1.0	–	0.0193	1.0	15–750	0.98	–	0.028	0.96	16–100	–	0.0173	1.0	500–1,500	Initial size of particle of explosive	p , atm.	$m (\delta)$						~5 μ	52	δ	0.50	0.51	0.66	0.73	0.88	$m (\text{g cm}^{-2} \text{ s}^{-1})$	0.99	0.85	0.86	0.88	0.99	100–400 μ	52	δ	0.60	0.82	0.86	0.90	–	$m (\text{g cm}^{-2} \text{ s}^{-1})$	0.99	1.00	0.87	0.99	–														
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Solubility [g/mL]	<p>Solubility, g PETN per 100 g (%) of^[13]:</p> <table><tr><th colspan="2">Trichloroethylene or alcohol</th><th colspan="2">Acetone</th><th colspan="2">Benzene</th><th colspan="2">Toluene</th></tr><tr><th>$T^\circ\text{C}$</th><th>%</th><th>$T^\circ\text{C}$</th><th>%</th><th>$T^\circ\text{C}$</th><th>%</th><th>$T^\circ\text{C}$</th><th>%</th></tr><tr><td>0</td><td>0.070</td><td>0</td><td>14.37</td><td>0</td><td>0.150</td><td>0</td><td>0.150</td></tr><tr><td>20</td><td>0.195</td><td>20</td><td>24.95</td><td>20</td><td>0.450</td><td>20</td><td>0.430</td></tr><tr><td>40</td><td>0.415</td><td>40</td><td>30.56</td><td>40</td><td>1.160</td><td>40</td><td>0.620</td></tr><tr><td>60</td><td>1.205</td><td>60</td><td>42.68</td><td>80</td><td>7.900</td><td>60</td><td>2.490</td></tr><tr><td></td><td></td><td></td><td></td><td></td><td></td><td>80</td><td>5.850</td></tr><tr><td></td><td></td><td></td><td></td><td></td><td></td><td>100</td><td>15.920</td></tr><tr><td></td><td></td><td></td><td></td><td></td><td></td><td>112</td><td>30.900</td></tr></table>	Trichloroethylene or alcohol		Acetone		Benzene		Toluene		$T^\circ\text{C}$	%	$T^\circ\text{C}$	%	$T^\circ\text{C}$	%	$T^\circ\text{C}$	%	0	0.070	0	14.37	0	0.150	0	0.150	20	0.195	20	24.95	20	0.450	20	0.430	40	0.415	40	30.56	40	1.160	40	0.620	60	1.205	60	42.68	80	7.900	60	2.490							80	5.850							100	15.920							112	30.900
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Solubility, g PETN per 100 g (%); eutectic of the system PETN–TNT is about 13% PETN and 87% TNT @ 76 °C^[13]:

Isopropanol		Isobutanol		Chloroform		TNT	
T°C	%	T°C	%	T°C	%	T°C	%
15	0.02	20	0.27	20	0.09	80	19.3
20	0.04	30	0.31			85	25.0
30	0.15	40	0.39			90	32.1
40	0.36	50	0.52			95	39.5
50	0.46					100	48.6
						105	58.2
						110	70.0
						115	87.8
						120	115
						125	161

Solubility, g PETN per 100 g (%)^[13]:

Methyl acetate		Ether		β-Ethoxy-ethyl-acetate		Chlorobenzene	
T°C	%	T°C	%	T°C	%	T°C	%
20	13	0	0.200	20	1.5	20	0.35
30	17	20	0.340	30	4.1	30	2.8
40	22	34.7	0.450	40	7.6	40	6.1
50	31			50	11.2	50	9.2
				60	14.2	60	12.2

Ethylenedi-chloride		Methanol		Tetrachloro-ethane		Carbon tetrachloride	
T°C	%	T°C	%	T°C	%	T°C	%
10	0.9	20	0.26	20	0.18	20	0.096
30	1.5	40	1.15	30	0.27	30	0.108
50	2.6	60	2.6	40	0.40	40	0.118
				50	0.58	50	0.121

0.0043 g/100 g H₂O @ 25 °C^[20], 0.018 g/100 g H₂O @ 96 °C^[20]

Solubility of PETN in acetone/water mixtures^[20]:

Amount of PETN (g) dissolved in 100 g solvent	Acetone concentration				
	55%	70%	80%	90%	92%
	T of soln. (°C)				
1	41				
2	52				
2.5		24.5			
4	62				
5		41.5	22		
10		54.5	38.5	15	10
15		62	48	24.5	20.5
17.5		65			
20			54	34.5	29
25			59	41.5	34
30			63	46.5	40.5
35				51.5	45
40				55	50
45				58.5	54
50				61.5	57.5
55					60.5
60					62.5

Data from^[21]:

Solvent	g dissolved/100 g solvent		
	20 °C	40 °C	60 °C
Acetone	24.8	44.92	—
Acetone and water (wt.% water)			
6.23	16.29	31.42	—
12.30	9.31	20.25	—
18.22	5.22	12.66	—
23.99	2.87	7.66	—
35.11	0.68	2.33	—
55.80	0.03	0.13	—
Benzene	0.27	0.83	2.58
EtOH	0.13	0.37	1.19
Ethyl acetate	10.6	18.50	—

Practically insoluble in H_2O ^[63, 107], 0.01 g in 100 g H_2O @ 50 °C^[63], 0.035 g in 100 g H_2O @ 100 °C^[63], soluble in most common organic solvents^[63], 24.6 g PETN per 100 g acetone @ 293 K^[88], 10.6 g PETN per 100 g ethyl acetate @ 293 K^[88], aqueous solubility = 2.1 mg/L @ 25 °C^[99], very slightly soluble in MeOH, EtOH, Et_2O , CCl_4 and cyclohexanol^[107], slightly soluble in hot EtOH, hot toluene and hot benzene^[107], very soluble in acetone and methyl acetate^[107], values of 2.1–43 mg/L in H_2O @ 25 °C are cited in the lit.^[111]

Solubility values from^[63]:

T (°C)	PETN (g) dissolved in 100 g solvent				
	EtOH	Et_2O	Acetone	Benzene	Toluene
0	0.070	0.200	14.37	–	0.150
10	0.085	0.225	16.43	0.150	0.170
20	0.115	0.250	20.26	0.200	0.230
30	0.275	0.340	24.95	0.450	0.430
40	0.415	0.450	36.16	1.60	0.620
50	0.705	–	–	2.010	1.100
60	1.205	–	–	3.350	2.490
62	–	–	42.68	–	–
70	2.225	–	–	5.400	3.290
78.4	3.795	–	–	5.400	–
80.2	–	–	–	7.900	–
90	–	–	–	–	9.120
113	–	–	–	–	30.960

Values taken from^[63]: 6.322 g soluble in 100 g ethyl acetate @ 19 °C^[63], 17.868 g soluble in 100 g ethyl acetate @ 50 °C^[63], 5.436 g soluble in 100 g pyridine @ 19 °C^[63], 8.567 g soluble in 100 g pyridine @ 50 °C^[63]

Solubility in acetone/ H_2O mixtures (amount of PETN (g) dissolved in 100 g solvent mixture/acetone concentration/T (°C))^[63]:
 1 g/55%/41 °C, 2/55/52, 4/55/62, 2.5/70/24.5, 5/70/41.5, 10/70/54.5, 15/70/62, 17.5/70/65, 5/80/22, 10/80/38.5, 15/80/48, 20/80/54, 25/80/59, 30/80/63, 10/90/15, 15/90/24.5, 20/90/34.5, 25/90/41.5, 30/90/46.5, 35/90/51.5, 40/90/55, 45/90/58.5, 50/90/61.5, 10/92/10, 15/92/20.5, 20/92/29, 25/92/34, 30/92/40.5, 35/92/45, 40/92/50, 45/92/54, 50/92/57.5, 55/92/60.5, 60/92/62.5^[63]

g PETN dissolved in 100 g solvent, values from^[63]:

$T(^{\circ}\text{C})$	Acetone	Benzene	EtOH
15	20.81	–	–
20	24.84	0.275	0.125
25	30.56	–	–
30	34.56	0.496	0.213
40	44.93	0.834	0.378
50	58.76	1.448	0.657
60	–	2.389	1.196

DMF: 40 g PETN dissolves in 100 g DMF @ 40 °C^[63], 50 g PETN dissolves in 100 g DMF @ 60 °C^[63], 70 g PETN dissolves in 100 g DMF @ 100 °C^[63],

1 part PETN dissolves in 18 parts H₂O @ 15 °C^[64], insoluble in H₂O^[102], soluble in acetone and methyl acetate^[102], solubility in H₂O = 0.01% @ 19 °C^[117], 0.035% @ 100 °C^[117]

Data from^[117]:

$T(^{\circ}\text{C})$	Solubility of PETN (g) per 100 g solvent				
	MeOH	EtOH	Et ₂ O	Benzene	Toluene
0	0.19	0.07	0.20		0.15
10	0.24	0.08	0.22	0.15	0.17
20	0.45	0.16	0.25	0.30	0.23
30	0.71	0.27	0.34	0.45	0.43
35			0.45		
40	1.16	0.42		1.16	0.62
50	1.8	0.71		2.01	1.10
60	2.60	1.21		3.35	2.49
62					
65	3.24				
70		2.22		5.40	3.29
74		3.79			
80				7.90	5.85
90					9.12
100					15.92
113					30.69

Data from^[117]:

T (°C)	Solubility of PETN (g) in 100 g solvent						
	Cello- solve	Methyl cello- solve	Car- bitol	Methyl carbitol	Carbitol acetates	Butyl carbitol	DMF
25	1.1	1.8	0.9	1.5	3.0	0.8	26.4
100	24.6	33.1	19.3	25.4	32.5	15.8	42.6

Solubility of PETN (g) in 100 g acetone containing various quantities of water (g)^[117]:

T (°C)	Solubility of PETN (g) in 100 g acetone containing various quantities of water (g)						
	0	2.5	6.25	9.07	10.0	14.29	30
10					16.4		
25	31.4	25.6		20.0	22.0	9.4	3.4
45	50.6		33.7	29.9	33.0	22.1	
55	66.6	60.0	46.0		37.5	30.7	9.7
62					42.7		

Almost insoluble in water^[138], soluble in acetone, methyl acetate^[138], insoluble in EtOH, Et₂O^[138], can form eutectic with NG^[138]

Solubility of PETN in TNT @ different T (g PETN/100 g TNT)^[138]:

T (°C)	g PETN/100 g TNT
80	19.3
85	25.0
90	32.1
95	39.5
100	48.6
105	58.2
110	70.0
115	87.8
120	115.0
125	161.0

Data from ^[138] ;		PETN dissolution capability of solvent (100 mL) at different <i>T</i> (°C)											
Solvent	0	20	25	30	40	47	50	60	80	100			
Acetone	14.37	24.95	–	–	30.56	–	–	42.68	–	–			
Benzene	0.15	0.45	–	–	1.16	–	–	3.35	–	–			
β-Ethoxyethyl acetate	–	1.5	–	4.1	7.6	–	11.2	14.2	–	–			
CCl ₄	–	0.096	–	0.108	0.118	–	0.121	–	–	–			
CHCl ₃	–	0.09	–	–	–	–	–	–	–	–			
Ethylene epoxide	–	0.35	–	2.8	6.1	–	9.2	12.2	–	–			
Ethyl ether	0.20	0.34	–	–	–	0.45	–	–	–	–			
EtOH	0.07	0.195	–	–	0.415	–	–	11.6 (61 °C)	–	–			
Dichloroethane	–	0.9 (10 °C)	–	1.25	5.02 (43 °C)	–	8.28	13.8 (65 °C)	–	–			
MeOH	–	0.46	–	–	1.15	–	–	2.60	–	–			
Ethyl formate	–	13.0	–	17.0	22.0	–	31.0	–	–	–			
Ethyl acetate	–	6.322 (19 °C)	–	–	–	–	17.863	–	–	–			
2-Methyl-1-propanol	–	0.27	–	0.31	0.39	–	0.52	–	–	–			
Nitromethane	3.36	–	8.89	–	–	–	–	–	8.89	–			
Tetrachloroethane	–	0.18	–	0.27	0.40	–	0.58	–	–	–			
Toluene	0.15	0.43	–	–	0.62	–	–	2.49	–	15.92			
DMF	–	–	–	–	40	–	–	50	–	70			
Pyridine	–	5.436 (19 °C)	–	–	–	–	8.567	–	–	–			

Hygroscopicity	0.0% @ 30 °C with 90% RH ^[13] , completely nonhygroscopic ^[63] , nonhygroscopic and not affected by moisture ^[102] , nonhygroscopic ^[117] , does not adsorb water ^[138]																																																										
Radiation sensitivity	<p>Effect of UV light on the thermal dec. of PETN/grit samples; PETN/additive samples were irradiated with UV light as they were being heated in the TC; reaction parameters in the presence of UV light^[55]:</p> <table><tr><th>Sample</th><th>E_a (kJ/mol)</th><th>$\ln A_s$</th><th>E_d (kJ/mol)</th><th>$\ln A_d/\ln (s^{-1})$</th><th>T_p (K)</th></tr><tr><td>PETN</td><td>143 ± 5</td><td>31 ± 4</td><td>193 ± 7</td><td>44 ± 6</td><td>478</td></tr><tr><td>PETN + UV</td><td>120 ± 4</td><td>28 ± 2</td><td>183 ± 16</td><td>45 ± 4.5</td><td>458</td></tr><tr><td>PETN, PC + UV</td><td>124 ± 8</td><td>29 ± 3</td><td>196 ± 25</td><td>49 ± 7</td><td>458</td></tr><tr><td>PETN, PP + UV</td><td>102 ± 8</td><td>22 ± 4</td><td>186 ± 8</td><td>45 ± 3</td><td>458</td></tr><tr><td>PETN, PS + UV</td><td>112 ± 8</td><td>25 ± 2.5</td><td>E_{d1} 368 ± 9 E_{d2} 185 ± 15</td><td>$\ln A_{d1}$ 99 ± 6 $\ln A_{d2}$ 47 ± 5</td><td>446</td></tr></table> <p>Decomposed by irradiation with γ-rays^[63], PETN (heated to just above its mpt.) explodes on exposure for 20 μs to irradiation producing 480 J energy^[63], quick dec. occurs if crystal exposed for 1.2 ms to intensive UV irradiation of 900 J energy^[63]</p> <p>significant drop in chemical stability after exposure to γ-rays with intensity of 3×10^4 Roentgens/h; administering doses of 3 megareoentgens reduced its stability to zero (cobalt-60 source)^[107], PETN phlegmatized with paraffin shows considerably higher resistance showing stability even with doses of 20 megareoentgens^[107]</p> <p>Data obtained from explosives after exposure to gamma radiation^[119]:</p> <table><tr><td>Weight of sample</td><td>5</td></tr><tr><td colspan="2">Volume of gas produced (mL/g) in following time (days)</td></tr><tr><td>10</td><td>0.10</td></tr><tr><td>20</td><td>0.43</td></tr><tr><td>30</td><td>1.04</td></tr><tr><td>40</td><td>2.33</td></tr><tr><td>50</td><td>–</td></tr><tr><td>90</td><td>–</td></tr><tr><td>Total irradiation time (days)</td><td>42</td></tr><tr><td>mpt. (°C) original material</td><td>140.8</td></tr><tr><td>mpt. (°C) irradiated sample</td><td>137.0</td></tr></table>	Sample	E_a (kJ/mol)	$\ln A_s$	E_d (kJ/mol)	$\ln A_d/\ln (s^{-1})$	T_p (K)	PETN	143 ± 5	31 ± 4	193 ± 7	44 ± 6	478	PETN + UV	120 ± 4	28 ± 2	183 ± 16	45 ± 4.5	458	PETN, PC + UV	124 ± 8	29 ± 3	196 ± 25	49 ± 7	458	PETN, PP + UV	102 ± 8	22 ± 4	186 ± 8	45 ± 3	458	PETN, PS + UV	112 ± 8	25 ± 2.5	E_{d1} 368 ± 9 E_{d2} 185 ± 15	$\ln A_{d1}$ 99 ± 6 $\ln A_{d2}$ 47 ± 5	446	Weight of sample	5	Volume of gas produced (mL/g) in following time (days)		10	0.10	20	0.43	30	1.04	40	2.33	50	–	90	–	Total irradiation time (days)	42	mpt. (°C) original material	140.8	mpt. (°C) irradiated sample	137.0
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PETN irradiated at ambient T using $0.41 \text{ MeV } ^{198}_{79}\text{Au } \gamma$ -rays; volumes of gas produced measured during and after irradiation, amount of gas evolved as function of gamma dose^[137]:

Gamma energy absorbed, 10^7 R	Gas evolved (mL/g) @ STP
1	0.1
2	0.5
3	1
4	2

Effect of 60 MeV electron irradiation on explosives^[137]:

Weight (mg)	Dose (R)	Dose rate (R/s)	Weight loss	Color change	Test	Results
14.0	1.14×10^9	0.6×10^6	None	Gray	Heat	Sample evaporated

Critical doses and T to initiate PETN by pulsed high-energy electrons, ^a = estimated 50% initiation dose^[137]:

Explosive	Critical dose (J/g)		Ignition T (°C)	
	Calcd.	Exptl. ^a	Calcd.	Exptl.
PETN	89.6	> 167	222	205 - 225

UV rays can detonate PETN^[138], rapid dec. and explosion on strong radiation for 1.2 ms with UV (900 J)^[138], can explode within 20 ms of UV radiation with 480 J^[138]

Data from^[143]:

Exposure rate (R/h)	Total dose (R)	Vacuum stability test		
		100 °C (cc/g/40 h)	120 °C (cc/g/40 h)	200 °C (cc/.2 g/2 h)
	Control	0.45	1.54	Deflagrated (88 min)
6.4×10^5	1.0×10^7	4.43	11 + (6 h)	Deflagrated (3 min)
	9.0×10^7	11+ (30 min)		

DTA for irradiated DATB @ 20 °C/min^[143]:

Total dose (R)	Endotherms				Exotherms			
	1st		2nd		1st		2nd	
	Onset (°C)	Peak (°C)	Onset (°C)	Peak (°C)	Onset (°C)	Peak (°C)	Onset (°C)	Peak (°C)
0	183	143			160	216		
1.0×10^7	127	133	136	141	170	215		
9.0×10^7	115	138			160	215		
1.06×10^9					130	163	187	242

TGA for irradiated DATB^[143]:

Total dose (R)	Heating rate (°C/min)	Weight (mg)	Start of dec. (°C)	10% Weight loss T (°C)	Total weight loss (%)	Remarks
0	20	8.3	160	187	96 @ 220 °C	–
1.0×10^7	20	8.4	135	178		–
9.0×10^7	20	8.15	70	177	96 @ 220 °C	–
0	50	8.45	173	200	46 @ 219 °C	Deflagrated @ 219 °C
1.0×10^7	50	8.5	130	197	30 @ 212 °C	Deflagrated @ 212 °C
9.0×10^7	50	8.5	70	184	50 @ 214 °C	Deflagrated @ 214 °C

Effect of gamma radiation on the mpt. and color^[143]:

Total dose (R)	mpt. (°C)	Color
0	141.5	White
1.0×10^7	141.5	White
9.0×10^7	136	White
1.06×10^9		White paste

IS for irradiated explosives, 50% fire height in inches, Bruceton method (P.A. apparatus, 2 kg mass)^[143]:

Total Co ⁶⁰ gamma dose (R)	\bar{X} mean (in)	σ std. dev. (in)
0	9.23	4.47
1.0×10^7	7.69	3.28
9.0×10^7	7.56	7.45

Effect of gamma radiation on explosion T (5 s explosion T in °C) and activation energy (kcal/mol)^[143]:

Total dose (R)	5 s explosion T (°C)	Apparent activation energy (kcal/mol)
0	228	18.12
9.0×10^7	222	14.16

Effect of gamma radiation on rates of detonation^[143]:

Total dose (R)	Density (g/cc)	Density after irradiation (g/cc)	Rate of detonation (m/s)	Detonation pressure (kbar)
0	1.67	—	8,045	270
1.0×10^7	1.68	1.67	8,035	270
9.0×10^7	1.66	1.54	7,660	226
$X \cdot 10 \times 10^9$	1.66	Pellets crumbled		

*X = illegible in original literature

Compatibility

Dry PETN does not affect: Cu, brass, Al, Mg, Mg-Al alloy, stainless steel, mild steel, mild steel coated with acid-proof black paint or mild steel plated with Cu, Cd, Ni or Zn^[13], wet PETN does not affect: stainless steel and Al is only slightly affected after prolonged storage^[13, 20], wet PETN affects: Cu, brass, Mg, Mg-Al alloy, mild steel, mild steel coated with acid-proof black paint or mild steel plated with Cu, Cd, Ni or Zn^[13, 20], nonhygroscopic and not affected by moisture^[102], reacts to some extent with most metals when wet^[102], most metals unaffected by dry PETN^[102], slowly dec. by caustic soda^[102], rapid dec. in soln. of boiling ferrous chloride^[102], dry PETN does not corrode metals at normal or elevated T ^[107], in presence of moisture slight corrosion of brass, cadmium or zinc occurs^[107], several hours required for dec. by boiling in 2.5% aq. NaOH soln.^[20], hydrolysis in water @ ~100 °C^[20], rapid dec. @ 125 °C under pressure^[20], @ $T < 50$ °C dry PETN does not

	<p>react with Cu, brass, Al, Mg, Mg–Al alloys, stainless steel, mild steel, mild steel coated with acid-proof black paint and mild steel plated with Cu, Cd, Ni or Zn^[20], presence of >0.01% acid or alkali rapidly accelerate PETN dec.^[20], rapid increase in dec. occurs if 0.01% free acid or alkali is present @ 65 °C for 15 months^[20], dry PETN does not react with metals^[8], wet PETN reacts with Cu, brass, Mg, Mg–Al alloy, mild steel, mild steel coated with acid-proof black paint and mild steel plated with Cd, Cu, Cu, Ni or Zn^[8], wet PETN affects Al after prolonged exposure^[8], presence of only 0.01% free acid causes rapidly increasing dec.^[8], does not react with metal^[117], dec. after long-term reaction with bases and acids^[117], compatible with vaseline and paraffin^[117], storing cast mixture of PETN/TNT (50:50) for 3 years @ RT resulted in decrease in pH from 6.58 to 5.46^[117], stability of PETN also decreases when other nitro derivatives of benzene and toluene are added^[117]</p> <p>A = no reaction, B = slight reaction, C = reacts readily, D reacts to form sensitive materials, H = heavy corrosion of metals, VS = very slight corrosion of metals, S = slight corrosion of metals, N = no corrosion^[119]:</p> <table><tr><th>Material</th><th colspan="3">Compatibility</th></tr><tr><td>Magnesium</td><td>B</td><td>N</td><td>S</td></tr><tr><td>Aluminum</td><td>A</td><td>N</td><td>VS</td></tr><tr><td>Steel</td><td>B</td><td>N</td><td>VS</td></tr><tr><td>Copper</td><td>B</td><td>N</td><td>VS</td></tr><tr><td>Cadmium-plated steel</td><td>B</td><td>N</td><td>S</td></tr><tr><td>Copper-plated steel</td><td>B</td><td>N</td><td>VS</td></tr><tr><td>Nickel-plated steel</td><td>B</td><td>N</td><td>VS</td></tr><tr><td>Zinc-plated steel</td><td>B</td><td>N</td><td>VS</td></tr><tr><td>Magnesium aluminum</td><td>B</td><td>N</td><td>S</td></tr><tr><td>Brass</td><td>B</td><td>N</td><td>S</td></tr><tr><td>18–8 stainless steel</td><td>A</td><td>N</td><td>N</td></tr></table> <p>Acetone, acids and alkali can all accelerate the hydrolysis of PETN^[138], no weight loss of PETN after heating in water for 2 h @ 100 °C, but rapidly hydrolyzes @ 125 °C under pressure^[138]</p>	Material	Compatibility			Magnesium	B	N	S	Aluminum	A	N	VS	Steel	B	N	VS	Copper	B	N	VS	Cadmium-plated steel	B	N	S	Copper-plated steel	B	N	VS	Nickel-plated steel	B	N	VS	Zinc-plated steel	B	N	VS	Magnesium aluminum	B	N	S	Brass	B	N	S	18–8 stainless steel	A	N	N
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Dipole moment [D]	$\mu = \sim 2.0$ (dilute soln. of PETN in benzene) ^[63, 138] , 2.5 in 1,4-dioxocyclohexane ^[138]																																																
Specific heat [cal/g/°C]	0.26 @ RT ^[13] , 1.09 J g ⁻¹ K ⁻¹ (@ RT) ^[55] , 0.4 ^[63] , 0.272 ^[86] , 0.4 kcal/g/°C ^[117]																																																
Heat capacity [J/(g °C)]	Heat capacity @ constant pressure = 0.239 + 0.008 T cal/g-°C @ 32 < T < 127 °C ^[21] , 1.67 ^[138]																																																

Latent heat of sublimation [kcal/mol]	36.3 ± 0.5 ^[63] , 146.6 kJ/mol (ΔH_{sub}) ^[109] , 151.9 kJ/mol (enthalpy of subl.) ^[138] , 91.9 cal/g (latent heat of sublimation, 29.1 kcal/mol) ^[21]																																																						
Thermal conductivity [calcm ⁻¹ s ⁻¹ °C ⁻¹]	0.0006 ^[86]																																																						
Bourdon manometer [mL/g]	28.20 (120 °Cm 48 h) ^[79]																																																						
Cook-off temperature, T_c [°C]	145 (prior to cook-off melting occurs, after 5 minutes heating in molten state, explosive process develops within molten sample, heating rate = 1 °C/min until cook-off registered as temperature jump) ^[91]																																																						
Energy to dec. [J/g]	1,309 ^[96]																																																						
ΔH_{melt} [J/g]	-504.6 (heat absorption) ^[98] , 96.2–100.4 kJ/mol ^[138] , 11.82 kcal/mol (latent heat of melting, calcd. from vapor pressure data) ^[21]																																																						
Heat of fusion [cal/g]	<div>76^[99], 144.7 kJ/kg^[55], 48^[88], 10.0 cal g⁻¹ (latent heat of fusion)^[86]</div> <div>Heats of fusion of different PETN crystal habits determined by gas permeability^[101]:</div> <table><thead><tr><th>Habit</th><th>Surface (cm²/g)</th><th>ΔH_{fusion} (cal/g)</th></tr></thead><tbody><tr><td rowspan="3">Superfine</td><td>4,700</td><td>31.7 ± 0.1</td></tr><tr><td>4,300</td><td>31.8 ± 0.2</td></tr><tr><td>5,400</td><td>33.2 ± 0.2</td></tr><tr><td rowspan="4">Needle</td><td>3,250</td><td>36.5 ± 0.3</td></tr><tr><td>4,400</td><td>37.0 ± 0.1</td></tr><tr><td>16,400</td><td>36.6 ± 0.3</td></tr><tr><td>18,600</td><td>37.7 ± 1.2</td></tr><tr><td rowspan="3">Tetragonal</td><td>1,000</td><td>36.8 ± 0.4</td></tr><tr><td>1,000</td><td>36.5 ± 0.5</td></tr><tr><td>Single crystals</td><td>37.4 ± 0.3</td></tr></tbody></table> <div>DSC, flame sealed in glass microampoules, N₂ @ 50 mL/min^[109]:</div> <table><thead><tr><th>Heating rate (K/min)</th><th>ΔH_{fus} (J/g)</th><th>Heating rate (K/min)</th><th>ΔH_{fus} (J/g)</th></tr></thead><tbody><tr><td>20</td><td>109</td><td>5</td><td>110</td></tr><tr><td>10</td><td>148</td><td>4</td><td>117</td></tr><tr><td>9</td><td>128</td><td>3</td><td>102</td></tr><tr><td>8</td><td>147</td><td>2</td><td>120</td></tr><tr><td>7</td><td>145</td><td>1</td><td>137</td></tr><tr><td>6</td><td>117</td><td></td><td></td></tr></tbody></table>	Habit	Surface (cm ² /g)	ΔH_{fusion} (cal/g)	Superfine	4,700	31.7 ± 0.1	4,300	31.8 ± 0.2	5,400	33.2 ± 0.2	Needle	3,250	36.5 ± 0.3	4,400	37.0 ± 0.1	16,400	36.6 ± 0.3	18,600	37.7 ± 1.2	Tetragonal	1,000	36.8 ± 0.4	1,000	36.5 ± 0.5	Single crystals	37.4 ± 0.3	Heating rate (K/min)	ΔH_{fus} (J/g)	Heating rate (K/min)	ΔH_{fus} (J/g)	20	109	5	110	10	148	4	117	9	128	3	102	8	147	2	120	7	145	1	137	6	117		
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$\Delta H_{\text{dec.}}$ [J/g]	2,385 (heat release) ^[98] , heat of dec. = 234 cal/g (est.) ^[116] DSC, flame sealed in glass microampoules, N ₂ @ 50 mL/min ^[109] : <table><tr><th>Heating rate (K/min)</th><th><i>n</i></th><th>Mass (mg)</th><th>Exotherm, <i>T</i>_{min} (°C)</th><th>Exotherm, <i>T</i>_{max} (°C)</th><th>ΔH (J/g)</th></tr><tr><td>20</td><td>4</td><td>0.125</td><td>198</td><td>212</td><td>1,971</td></tr><tr><td>10</td><td>4</td><td>0.297</td><td>193</td><td>202</td><td>3,874</td></tr><tr><td>9</td><td>3</td><td>0.280</td><td>192</td><td>201</td><td>3,358</td></tr><tr><td>8</td><td>4</td><td>0.298</td><td>191</td><td>199</td><td>4,032</td></tr><tr><td>7</td><td>3</td><td>0.330</td><td>188</td><td>196</td><td>3,634</td></tr><tr><td>6</td><td>3</td><td>0.326</td><td>189</td><td>195</td><td>4,060</td></tr><tr><td>5</td><td>3</td><td>0.284</td><td>186</td><td>194</td><td>3,734</td></tr><tr><td>4</td><td>3</td><td>0.289</td><td>183</td><td>192</td><td>2,985</td></tr><tr><td>3</td><td>3</td><td>0.282</td><td>181</td><td>189</td><td>2,919</td></tr><tr><td>2</td><td>3</td><td>0.301</td><td>178</td><td>183</td><td>3,553</td></tr><tr><td>1</td><td>3</td><td>0.352</td><td>172</td><td>173</td><td>4,096</td></tr></table>					Heating rate (K/min)	<i>n</i>	Mass (mg)	Exotherm, <i>T</i> _{min} (°C)	Exotherm, <i>T</i> _{max} (°C)	ΔH (J/g)	20	4	0.125	198	212	1,971	10	4	0.297	193	202	3,874	9	3	0.280	192	201	3,358	8	4	0.298	191	199	4,032	7	3	0.330	188	196	3,634	6	3	0.326	189	195	4,060	5	3	0.284	186	194	3,734	4	3	0.289	183	192	2,985	3	3	0.282	181	189	2,919	2	3	0.301	178	183	3,553	1	3	0.352	172	173	4,096
Heating rate (K/min)	<i>n</i>	Mass (mg)	Exotherm, <i>T</i> _{min} (°C)	Exotherm, <i>T</i> _{max} (°C)	ΔH (J/g)																																																																								
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Diffusion coefficient (air) [cm ² /s]	0.057 ^[99]																																																																												
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Log <i>K</i> _{ow}	3.71 ^[99, 111]																																																																												
Log <i>K</i> _{oc}	3.39 ^[99]																																																																												
Fracture surface energy [J m ⁻²]	≤0.11 ^[108]																																																																												
Hardness	1.9 (Moh's scale) ^[13] , 17.9 kg mm ⁻² (Vicker's hardness) ^[55, 108] , slightly less than 2 (Moh's scale, PETN crystals) ^[20] , 17.9 ± 0.6 kg mm ⁻² (single crystals, ~5 mm diameter, @ 20 °C, Vicker's hardness) ^[115] , 1.8 (Moh's scale) ^[119]																																																																												
Small-scale explosivity device (SSED)	British .303 cartridge, 2 g explosive, RP-3 EBW ^[109] : <table><tr><th>Charge depth (mm)</th><th>Tap density (g mL⁻¹)</th><th>Mass cartridge (g)</th><th>Mass remaining (g)</th><th>Fraction remaining (%)</th></tr><tr><td>17</td><td>0.69</td><td>11.0747</td><td>2.8792</td><td>26</td></tr><tr><td>14</td><td>0.64</td><td>11.183</td><td>2.9109</td><td>26</td></tr><tr><td>18</td><td>0.71</td><td>11.3524</td><td>3.0374</td><td>26.8</td></tr></table>					Charge depth (mm)	Tap density (g mL ⁻¹)	Mass cartridge (g)	Mass remaining (g)	Fraction remaining (%)	17	0.69	11.0747	2.8792	26	14	0.64	11.183	2.9109	26	18	0.71	11.3524	3.0374	26.8																																																				
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Rifle bullet impact test	100% explosions in five trials (4.86% moisture in samples) ^[13] , 100% explosions in tests ^[119] , 100 % detonations (pressed sample, Reg disk bomb, 3/16 in steel disk) ^[140]																																						
Plate dent test	<p>Brisance = 129% TNT, method A, pressed, confined, $\rho = 1.50 \text{ g cm}^{-3}$^[13], brisance = 127% TNT^[20]</p> <p>Data from^[21]:</p> <table><tr><td>Density (g/cm³)</td><td>Dent depth (mm)</td><td>Charge height (mm)</td></tr><tr><td>1.670</td><td>9.80</td><td>–</td></tr><tr><td>1.665</td><td>9.75</td><td>203</td></tr></table>							Density (g/cm ³)	Dent depth (mm)	Charge height (mm)	1.670	9.80	–	1.665	9.75	203																							
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1.670	9.80	–																																					
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Booster sensitivity test	Pressed, 5 g tetryl, 3 g wax, $\rho = 1.60 \text{ g cm}^{-3}$ ^[13, 119]																																						
Laser sensitivity	<p>PETN does not initiate with normal light except in few examples of deflagration with very intense light^[20], lasers can be used to initiate PETN^[20], 5 mm thick PETN ($\rho = 1.0 \text{ g cm}^{-3}$) initiated by neodymium glass laser with output @ 10,600 Å with focused beam producing power density >0.08 MW/mm², delay in ignition is 1.5–2.0 μs^[20], delay in ignition is <0.5 μs if PETN is coated with 1,000 Å thick layer of Al and laser radiation is from 0.5–4.2 J for 25 ns^[20], successful detonation, if PETN sample compressed against glass plate (Ruby laser (6,943 Å) both in free running and Q-switch modes)^[119]</p> <p>Detonation conditions using laser-produced heat and shock^[122]:</p> <table><tr><td>Den- sity</td><td>Deto- nator type</td><td>Nomi- nal wave- length (nm)</td><td>Spot diam- eter (mi- crons)</td><td>Power or energy (J)</td><td>Func- tion time (μs)</td><td>Laser type</td><td>Pulse dura- tion (μs)</td></tr><tr><td>1.64</td><td>Uncon- fined</td><td>1,060</td><td>600</td><td>0.26</td><td></td><td>Neo- dymium/ glass</td><td>250</td></tr><tr><td>1.64</td><td>Con- fined</td><td>694</td><td>< 3,000</td><td>1</td><td>2.9</td><td>Q- switched ruby</td><td>0.43</td></tr><tr><td>1.72</td><td>Con- fined</td><td>694</td><td>< 3,000</td><td>2</td><td>2.9</td><td>Q- switched ruby</td><td>0.36</td></tr></table>							Den- sity	Deto- nator type	Nomi- nal wave- length (nm)	Spot diam- eter (mi- crons)	Power or energy (J)	Func- tion time (μs)	Laser type	Pulse dura- tion (μs)	1.64	Uncon- fined	1,060	600	0.26		Neo- dymium/ glass	250	1.64	Con- fined	694	< 3,000	1	2.9	Q- switched ruby	0.43	1.72	Con- fined	694	< 3,000	2	2.9	Q- switched ruby	0.36
Den- sity	Deto- nator type	Nomi- nal wave- length (nm)	Spot diam- eter (mi- crons)	Power or energy (J)	Func- tion time (μs)	Laser type	Pulse dura- tion (μs)																																
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	Initiation energy of PETN using free-running laser; X = ignition, O = no ignition ^[123] ; <table><tr><td>Energy range (J/sq mm)</td><td>Detonation</td></tr><tr><td>0.0795–0.1000</td><td>O X</td></tr><tr><td>0.1001–0.1260</td><td>O</td></tr><tr><td>0.1261–0.1590</td><td>O</td></tr><tr><td>0.1591–0.2000</td><td>O X X</td></tr><tr><td>0.2001–0.2510</td><td>O X</td></tr><tr><td>0.2511–0.3160</td><td>X X</td></tr><tr><td>0.3161–0.3980</td><td>X</td></tr></table>	Energy range (J/sq mm)	Detonation	0.0795–0.1000	O X	0.1001–0.1260	O	0.1261–0.1590	O	0.1591–0.2000	O X X	0.2001–0.2510	O X	0.2511–0.3160	X X	0.3161–0.3980	X
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0.2511–0.3160	X X																
0.3161–0.3980	X																
Frictional properties	Frictional properties @ 20 °C with sliding velocity of 0.20 mms ⁻¹ ^[115] ; <table><tr><td>μ (coef- ficient of friction at high loads)</td><td>τ_0 (constant)</td><td>α (constant)</td><td>μ_{cal} (calcd. coefficient of friction at high loads)</td><td>μ (coefficient of friction for single crystal on single crystal)</td><td>-(l-m)</td></tr><tr><td>0.40</td><td>-5.0×10^5 Pa</td><td>0.45 ± 0.05</td><td>0.38 ± 0.02</td><td>0.40</td><td>0.39</td></tr></table>	μ (coef- ficient of friction at high loads)	τ_0 (constant)	α (constant)	μ_{cal} (calcd. coefficient of friction at high loads)	μ (coefficient of friction for single crystal on single crystal)	-(l-m)	0.40	-5.0×10^5 Pa	0.45 ± 0.05	0.38 ± 0.02	0.40	0.39				
μ (coef- ficient of friction at high loads)	τ_0 (constant)	α (constant)	μ_{cal} (calcd. coefficient of friction at high loads)	μ (coefficient of friction for single crystal on single crystal)	-(l-m)												
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Critical air gap	0.47 in (0.2 in diameter) ^[119]																
Reflectance tests	Reflectance tests @ 10,600 Å (continuous wave yttrium garnet aluminum laser, pressed explosive) ^[121] ; <table><tr><td>Particle size, mesh</td><td>Loading pressure, 10³ psi</td><td>Reflectance, %</td></tr><tr><td>Class 1</td><td>10</td><td>88.5</td></tr><tr><td>Class 4</td><td>10</td><td>71.0</td></tr></table>	Particle size, mesh	Loading pressure, 10 ³ psi	Reflectance, %	Class 1	10	88.5	Class 4	10	71.0							
Particle size, mesh	Loading pressure, 10 ³ psi	Reflectance, %															
Class 1	10	88.5															
Class 4	10	71.0															
CRT	0.4–0.56 cm ³ /g (22 h @ 120 °C under 1 atm. He) ^[128]																
Shock sensitivity	Short pulse shock test (exploding foil), PETN class 2: threshold flyer velocity = 2.21 km/s, $\rho = 1.50$ g cm ⁻³ , consolidation pressure = 103.4 MPa ^[132]																
Small-scale shock reactivity test (SSRT)	Used sample weight = 482 mg, dent = 917 mg SiO ₂ ^[136]																
Abel test	Up to several hours ^[138]																

Flame sensitivity	Low, difficult to ignite with a flame ^[138] , seamless steel tube with 18 mm diameter loaded with PETN cannot be ignited, must be heated >95 °C to cause ignition ^[138]																	
Refractive index	Form I = α-PETN, form II = β-PETN ^[21] : <table><tr><td></td><td>Form I</td><td>Form II</td></tr><tr><td>Omega</td><td>1.556</td><td>1.556</td></tr><tr><td>Epsilon</td><td>1.551</td><td>1.551</td></tr><tr><td>Birefringence</td><td>0.005</td><td>0.002</td></tr><tr><td>Double refraction</td><td>Negative</td><td>–</td></tr></table>				Form I	Form II	Omega	1.556	1.556	Epsilon	1.551	1.551	Birefringence	0.005	0.002	Double refraction	Negative	–
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Cylinder test	Data from ^[21] : <table><tr><th rowspan="2">Density (g/cm³)</th><th rowspan="2">Detonation velocity (mm/μs)</th><th colspan="2">Cylinder wall velocity (mm/μs) at</th></tr><tr><th>R–R₀ = 5 mm</th><th>R–R₀ = 19 mm</th></tr><tr><td>1.765</td><td>8.16</td><td>1.56</td><td>1.79</td></tr></table>			Density (g/cm³)	Detonation velocity (mm/μs)	Cylinder wall velocity (mm/μs) at		R–R ₀ = 5 mm	R–R ₀ = 19 mm	1.765	8.16	1.56	1.79					
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Wedge test	Data from ^[21] : <table><tr><th>Density (g/cm³)</th><th>Distance, x* and time, t* to detonation (mm and μs)</th><th>Valid pressure range (GPa)</th></tr><tr><td>1.4</td><td>log P = (0.14 ± 0.03)–(0.4 ± 0.05) log x* log P = (0.04 ± 0.02)–(0.33 ± 0.04) log t*</td><td>0.66 < P < 0.99</td></tr><tr><td>1.6</td><td>log P = (0.40 ± 0.03)–(0.54 ± 0.05) log x* log P = (0.18 ± 0.02)–(0.44 ± 0.09) log t*</td><td>1.2 < P < 2.0</td></tr><tr><td>1.72</td><td>log P = (0.61 ± 0.03)–(0.49 ± 0.05) log x* log P = (0.34 ± 0.02)–(0.50 ± 0.09) log t*</td><td>1.7 < P < 3.9</td></tr><tr><td>1.75</td><td>log P = (0.57 ± 0.04)–(0.41 ± 0.06) log x* log P = (0.33 ± 0.02)–(0.22 ± 0.16) log t*</td><td>1.7 < P < 2.54</td></tr></table> <p>where P = pressure in GPa</p>			Density (g/cm³)	Distance, x* and time, t* to detonation (mm and μs)	Valid pressure range (GPa)	1.4	log P = (0.14 ± 0.03)–(0.4 ± 0.05) log x* log P = (0.04 ± 0.02)–(0.33 ± 0.04) log t*	0.66 < P < 0.99	1.6	log P = (0.40 ± 0.03)–(0.54 ± 0.05) log x* log P = (0.18 ± 0.02)–(0.44 ± 0.09) log t*	1.2 < P < 2.0	1.72	log P = (0.61 ± 0.03)–(0.49 ± 0.05) log x* log P = (0.34 ± 0.02)–(0.50 ± 0.09) log t*	1.7 < P < 3.9	1.75	log P = (0.57 ± 0.04)–(0.41 ± 0.06) log x* log P = (0.33 ± 0.02)–(0.22 ± 0.16) log t*	1.7 < P < 2.54
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VoD of foamed PETN (PETN was uniformly dispersed in polyurethane forms to achieve low densities):
 1.17 km/s @ 0.133 g cm⁻³^[23], 1.14 km/s @ 0.120 g cm⁻³^[23], 1.12 km/s @ 0.109 g cm⁻³^[23], 0.98 km/s
 @ 0.094 g cm⁻³^[23], 0.78 km/s @ 0.055 g cm⁻³^[23], 0.59 km/s @ 0.049 g cm⁻³^[23]

Additional exptl. VoD for PETN^[27, 40]:

VoD (mm/ μ s)	ρ (g cm ⁻³)	VoD (mm/ μ s)	ρ (g cm ⁻³)
8.60	1.77	7.42	1.51
8.35	1.73	6.97	1.37
7.98	1.67	5.62	1.03
8.10	1.66	5.33	0.97
7.92	1.65	5.30	0.95
7.91	1.62		

Exptl. VoD values, PETN particle diameter = 10 microns, charge diameter = 1.92 cm, average VoD for station distance of 10 cm^[35]:

VoD (m/s)	ρ (g cm ⁻³)
4,120	0.60
4,310	0.68
5,240	0.95
6,510	1.21
7,560	1.55

Radiation T observed without slit aperture, for interval after detonation of 18 μ s, loading $\rho = 1.64$ g cm⁻³, average $T = 6,220$ K^[35].

Additional VoD for PETN, pin switch measurements (a) = unconfined rate stick; (b) = cylinder test^[28]:

VoD (mm/ μ s)	ρ (gcm ⁻³)	VoD (mm/ μ s)	ρ (gcm ⁻³)
8.30	1.773 ^(a)	7.49	1.51 ^(b)
8.28	1.765 ^(b)	6.67	1.27 ^(b)
8.16	1.765 ^(b)	6.76	1.26 ^(b)
8.24	1.765 ^(a)	5.83	1.09 ^(b)
8.24	1.765 ^(a)	3.85	0.55 ^(a)
8.27	1.763 ^(a)	3.40	0.436
8.25	1.762 ^(a)	2.81	0.241 ^(a)
8.26	1.762 ^(a)	2.73	0.201 ^(a)
7.44	1.51 ^(b)	2.67	0.185 ^(a)

Additional VoD for PETN, shock electric effect measurements^[28]:

VoD (mm/ μ s)	ρ (gcm ⁻³)	VoD (mm/ μ s)	ρ (gcm ⁻³)
8.00	1.71	7.07	1.38
8.08	1.71	6.48	1.23
8.03	1.70	6.50	1.23
7.96	1.70	6.46	1.23
7.97	1.69	6.43	1.23
7.74	1.60	5.52	0.99
7.69	1.59	5.41	0.95
7.51	1.53	5.31	0.93
7.41	1.46	5.33	0.93
7.26	1.45	5.20	0.89
7.20	1.44	5.17	0.88

Additional VoD for PETN^[28]:

VoD (km/s)	ρ (g cm ⁻³)	VoD (km/s)	ρ (g cm ⁻³)
6.97	1.37	4.71	0.75
6.36	1.22	3.90	0.50
5.62	1.03	3.97	0.50
5.55	1.00	3.53	0.32
5.33	0.97	3.55	0.30
5.30	0.95	3.42	0.30
4.76	0.80	3.20	0.24

Additional VoD for PETN of two different particle sizes; charge diameter=0.32 cm^[28]: packing density=0.95 g cm⁻³, PETN of -35 \pm 48 mesh, VoD=4,300 m/s^[28], packing density=0.95 g cm⁻³, PETN of -65 \pm 100 mesh, VoD=4,800 m/s^[28], for a charge diameter of 0.63 cm, no difference in VoD observed for the two particle sizes^[28]

VoD can be increased by replacing air among crystals by a non-explosive liquid such as H_2O ^[63]:

PETN sample	Loading ρ (g cm^{-3})	VoD (m/s)
Dry PETN	1.45	7,295
PETN with 10% H_2O	1.45	7,445
Dry PETN	1.40	7,125
PETN with 10% H_2O	1.40	7,825

Values calculated for the detonation pressure and detonation temperature using hydrodynamic theory of detonation equations^[35]:

ρ of charge (g cm^{-3})	Detonation pressure (kg/cm^2)	Detonation temperature (K)
0.80	65,000	5,050
1.00	95,300	5,320
1.20	140,500	5,720
1.40	195,500	6,170
1.60	252,800	6,670

Calculated temperatures of detonation^[35]:

ρ of charge (g cm^{-3})	Average detonation temperature (K)
0.70	3,580
0.75	3,670
1.50	5,910
1.60	6,040

Exptl. determined temperatures of detonation (detonated in air at atmospheric pressure)^[35]:

ρ of charge (g cm^{-3})	Average detonation temperature (K)
0.68	3,750
0.95	4,020
1.55	6,460
1.68	5,840

Exptl. determined temperatures of detonation (detonated in glass cylinders)^[35]:

ρ of charge (g cm ⁻³)	Average detonation temperature (K)
0.70	4,980
0.95	4,960
1.60	5,520

Exptl. determined temperatures of detonation (within H₂O-filled glass cylinders)^[35]:

ρ of charge (g cm ⁻³)	Average detonation temperature (K)
0.60	4,080
0.95	3,970
1.55	5,650

Exptl. determined temperatures of detonation by radiation method (charges contained within evacuated glass cylinders)^[35]:

ρ of charge (g cm ⁻³)	Average detonation temperature (K)
0.82	5,590
1.55	5,230
1.60	5,330

Exptl. determined temperatures of detonation by radiation method (charges contained in H₂O-filled glass tubes)^[35]:

ρ of charge (g cm ⁻³)	Average detonation temperature (K)
0.72	4,020
0.98	3,990
1.44	5,350

Exptl. determined temperatures of detonation by luminosity method (unsheathed explosives in air)^[35]:

ρ of charge (g cm ⁻³)	Radiation slit width (mm)	Average detonation temperature (K)
1.18	1.0	6,000
1.64	1.0	5,750
1.60	1.5	5,450

VoD of PETN powder, charge diameter = 1.90 cm, station distance ca. 10 cm^[35]:

ρ (g cm ⁻³)	0.68	0.80	1.10	1.40	1.56
VoD (m/s)	4,160	4,730	5,990	7,270	7,445

PETN, confining vessel glass walls, 16 mm charge diameter, 0.8 mm wall thickness, charge density = 0.3 g cm⁻³, VoD = 3,419 m/s^[35]

PETN, confining vessel glass walls, 15 mm charge diameter, 1.0 mm wall thickness, charge density = 0.3 g cm⁻³, VoD = 3,548 m/s^[35]

Steady-state VoD measured in small, brass-confined pressings of PETN^[45]:

Diameter (mm)	$1/D$ (per mm) [reciprocal of charge diameter]	VoD (km/s)	Charge density (kg/m ³)
4.06	0.246	4.58	950
		4.56	950
		4.58	950
		4.60	950
7.62	0.131	4.88	950
		4.86	950
11.4	0.088	5.01	950
		5.02	950
14.0	0.071	5.06	950
		5.11	950
		4.80	900
		5.56	1,000
16.5	0.061	5.14	950

Detonation velocity of low-density foamed PETN charges, PMMA = polymethyl methacrylate, wall thickness ~6 mm, fine PETN has an average particle size of 10–12 microns^[103]:

Confinement		Type of PETN	Weight % PETN	Foam density, g/cc	Explosive density, g/cc	Detonation velocity, mm/ μ s
Type	I.D., cm					
PMMA	5.71	Coarse	Unknown	Unknown	0.185	2.15
PMMA	5.08	Fine	56.3	0.136	0.176	2.45

Steel	5.08	Fine	43.0	0.175	0.133	1.17
PMMA	5.08	Fine	43.8	0.154	0.120	1.14
Steel	5.08	Fine	47.4	0.121	0.109	1.12
Steel	5.08	Fine	39.8	0.142	0.094	0.98
Aluminum	5.08	Fine	40.2	0.087	0.058	1.02
PMMA	7.62	Fine	30.9	0.127	0.057	Unstable
Steel	5.08	Fine	31.0	0.124	0.055	0.78
PMMA	5.08	Fine	31.0	0.124	0.055	Unstable
Steel	5.08	Fine	30.7	0.112	0.049	0.59
Steel	5.08	Fine	13.3	0.140	0.022	Unstable

Calculation of detonation pressure for low-density foamed PETN charges, PMMA = polymethyl methacrylate^[103]:

Explosive density, g/cc	Foam density, g/cc	Minimum gage resistance, ohms	Gage pressure, kbars	PMMA pressure, kbars	Detonation pressure, kbars
0.176	0.136	274	7.6	8.0	4.8
0.133	0.175	282	7.1	7.5	—
0.101	0.086	331	4.4	4.9	—
0.058	0.087	381	2.4	2.9	—

Summary of calculated Chapman–Jouguet conditions for low-density explosive systems^[103]:

System	Initial explosive density, g/cc	Foam density, g/cc	CJ density, g/cc	CJ pressure, kbars	Particle velocity, mm/ μ s	γ
Foamed PETN	72	0.176	0.136	0.420	0.63	2.89
Expanded	106	0.252	—	0.550	1.02	0.84
	104	0.141	—	0.223	0.85	1.72
	105	0.104	—	0.141	0.54	2.84

PETN experimental detonation pressures from^[104]:

Density (g/cc)	Dimensions of PETN, diameter × length (in)	Detonation velocity (mm/μs)	Shock velocity (mm/μs)	Detonation pressure, P_{CJ} (kbar)
Shock electric effect measurements				
1.764	2 × 0.5	8.28	7.01	338
1.763	1 × 0.5	8.27	6.98	333
1.763	1 × 0.5	8.27	6.98	334
1.763	1 × 1	8.27	7.04	340
1.763	2 × 0.5	8.27	7.01	338
1.763	2 × 1	8.27	7.03	340
1.762	1 × 1	8.27	6.99	335
1.762	1 × 1	8.27	7.07	343
1.758	1 × 1	8.26	6.98	333
1.71	1 × 1	8.11	6.86	311
1.71	1 × 1	8.11	6.81	307
1.71	1 × 1	8.10	6.83	309
1.70	1 × 1	8.08	6.84	308
1.70	1 × 1	8.06	6.83	306
1.69	1 × 1	8.03	6.83	304
1.60	1 × 1	7.76	6.57	266
1.60	1 × 1	7.74	6.60	266
1.59	1 × 1	7.71	6.52	259
1.53	1 × 1	7.49	6.21	225
1.46	1 × 1	7.22	5.99	198
1.45	1 × 1	7.18	6.16	208
1.44	1 × 1	7.14	6.05	199
1.38	1 × 1	6.91	5.79	173
1.23	1 × 1	6.38	5.45	136
1.23	1 × 1	6.37	5.42	134
1.23	1 × 1	6.37	5.47	137
1.23	1 × 1	6.37	5.56	142

1.23	1 × 1	6.36	5.54	141
1.23	1 × 1	6.36	5.56	142
0.99	1 × 0.5	5.48	4.91	87
0.95	1 × 0.5	5.33	4.93	85
0.93	1 × 1.5	5.27	4.68	73
0.93	1 × 1	5.26	4.77	77
0.93	1 × 1.5	5.25	4.61	70
0.89	1 × 1	5.10	4.70	71
0.88	1 × 1	5.06	4.63	68
Optical (smear camera) measurements				
0.49	1.5 × 1	3.60	3.72	24
0.30	1.5 × 0.5	2.99	3.44	13
0.29	1.5 × 1	2.96	3.49	15
0.27	1.5 × 0.5	2.91	3.18	5
Quartz crystal measurements				
Density (g/cc)	Dimensions of PETN, diameter × length (in)	Detonation velocity (mm/μs)	Pressure in Quartz (kbar)	Detonation pressure, P_{CJ} (kbar)
0.25	1.75 × 1	2.83	16	8
0.25	1.75 × 1	2.83	13	7
0.25	1.75 × 1.5	2.83	12	6

PETN experimental detonation pressures, values cited in^[104]:

Density, g/cc	Detonation velocity, mm/μs	Detonation pressure, P_{CJ} , kbar
1.77	8.50	340
1.77	8.31	320
1.67	7.97	300
1.66	8.10	246
1.65	7.92	305
1.51	7.42	187
0.95	5.30	64

PETN experimental detonation velocities; * = unconfined rate stick, † = cylinder test, ‡ = detonation pressure experiments^[104]:

Density (g/cc)	Detonation velocity (mm/μs)	Density (g/cc)	Detonation velocity (mm/μs)
Pin switch measurement			
1.773	8.30*	1.27	6.66 [†]
1.765	8.28 [†]	1.26	6.76 [†]
1.765	8.16 [†]	1.09	5.83 [†]
1.765	8.24*	1.09	5.83 [†]
1.763	8.27*	0.55	3.85*
1.762	8.25*	0.436	3.40*
1.762	8.26*	0.241	2.81*
1.51	7.44 [†]	0.201	2.73*
1.51	7.49 [†]	0.185	2.67*
Shock electric effect measurement [‡]			
1.71	8.00	1.23	6.48
1.71	8.00	1.23	6.50
1.71	8.08	1.23	6.46
1.70	8.03	1.23	6.46
1.70	7.96	1.23	6.46
1.69	7.97	1.23	6.43
1.60	7.74	0.99	5.52
1.60	7.74	0.95	5.41
1.59	7.69	0.93	5.31
1.53	7.51	0.93	5.33
1.46	7.41	0.93	5.15
1.45	7.26	0.89	5.20
1.44	7.20	0.88	5.17
1.38	7.07		

Experimental detonation velocity values cited in^[104]:

Density (g/cc)	Detonation velocity (mm/ μ s)	Density (g/cc)	Detonation velocity (mm/ μ s)
1.77	8.50	1.03	5.62
1.73	8.35	1.00	5.55
1.67	7.97	0.97	5.33
1.66	8.10	0.95	5.30
1.65	7.92	0.95	5.35
1.62	7.91	0.80	4.76
1.60	7.92	0.75	4.71
1.51	7.42	0.50	3.90
1.51	7.42	0.50	3.97
1.40	7.13	0.32	3.53
1.37	6.97	0.30	3.55
1.22	6.36	0.3	3.42
1.20	6.34	0.24	3.20

Summary of experimental copper cylinder wall velocity data, samples have wall thickness/diameter ratio of 0.1 except those marked with an asterisk; all cylinders were 305 mm long, PETN with $\rho = 1.763 \text{ g/cm}^3$ is the reference explosive^[112]:

Initial density (g/cm ³)	Inner diameter (mm)	Wall thickness (mm)	Wall velocity (mm/ μ s) at 25.4 mm diameter for $R-R_0$ equal to			Velocity squared cf. with PETN for the same configuration, % comparison $R-R_0$ equal to		
			6 mm	12.5 mm	19 mm	6 mm	12.5 mm	19 mm
PETN (ref)	1.763	25.44	1.361*	2.285	2.415	0.0	0.0	0.0
PETN (ref)	1.763	25.43	2.594	1.560	1.790	0.0	0.0	0.0
PETN	1.507	25.45	1.365	1.832	2.125	-22.8	-20.3	-22.6
PETN	1.498	25.43	2.596	1.355	1.590	-24.6	-21.6	-21.1
PETN	1.266	25.42	2.598	1.156	1.382	-45.1	-41.5	-40.4
PETN	1.261	25.45	1.356	1.575	1.865	-42.9	-39.6	-40.4

Summary of code calculations with measured detonation velocities and detonation energies derived from JWL's data from ^[112]:

Explosive	Initial density (g/cm ³)	PETN-adjusted BKWR Tiger, LLNL library $\theta = 1,850$ K, at v			JCZ3, LLNL library, v			CHEQ V2.4, at v		
		2.2	4.1	6.5	2.2	4.1	6.5	2.2	4.1	6.5
PETN (ref)	1.763	0	0	0	-3	-4	-5	-9	-9	-9
PETN	1.503	0	-1	1	-4	-7	-5	-15	-14	12
PETN	1.263	1	0	2	-6	-8	-6	-18	-16	-13

Derivation of the total energy of detonation from the measured heat of detonation (the final state is assumed to at one atmosphere for all gaseous products, including water, at 298 K. Code calculated energies with the 1,800 K freeze)^[112]:

Measured density (g/cc)	Measured confined heat of detonation (kJ/cm ³)	Density from ^[112]	Heat of detonation using density from ^[112]	Energy of detonation E_0 (kJ/cm ³)			
				From heat of detonation	Freeze at 1,800 K		
					Tiger BKWR	Tiger JCZ3	CHEQ
1.732	-10.81	1.763	-11.01	-10.3	-10.7	-10.4	-10.5
1.496	-9.41	1.503	-9.46	-8.9	-9.0	-9.0	-8.7

JWL cylinder coefficients as determined in^[112]:

Initial density, ρ_0 (g/cm ³)	Detonation velocity, D (mm/ μ s)	Energy of detonation, E_0 (kJ/cm ³)	CJ pressure (GPa)	A (GPa)	B (GPa)	C (GPa)	R_1	R_2	ω	γ_{CJ}
1.763	8.274	-10.80	31.5	1,032.158	90.57014	3.72735	6.000	2.60	0.57	2.832
1.503	7.48	-8.50	24.9	351.0723	5.705547	1.216240	4.075	0.90	0.35	2.504
1.263	6.59	-7.20	16.0	228.1744	5.104579	1.412013	4.240	1.05	0.35	2.428

	PETN-I ^[20-22, 44]	PETN-II ^[21, 22, 44]	PETN ^[20, 22]	PETN ^[29]	PETN ^[30]	PETN ^[31]	PETN ^[32]
	Phase I (α -)	Phase I (β -)					
Chemical formula	C ₅ H ₈ N ₄ O ₁₂	C ₅ H ₈ N ₄ O ₁₂	C ₅ H ₈ N ₄ O ₁₂	C ₅ H ₈ N ₄ O ₁₂	C ₅ H ₈ N ₄ O ₁₂	C ₅ H ₈ N ₄ O ₁₂	C ₅ H ₈ N ₄ O ₁₂
Molecular weight [g mol ⁻¹]	316.14	316.14	316.14	316.14	316.14	316.14	316.14
Crystal system	Tetragonal	Orthorhombic	Orthorhombic	Tetragonal	Tetragonal	Tetragonal	Tetragonal
Space group	$P\bar{4}2_1c$ (no. 114)	$Pcnb$ (no. 60)	$Pcnb$ (no. 60)	$P\bar{4}2_1c$ (no. 114)	$P\bar{4}2_1c$ (no. 114)	$P\bar{4}2_1c$ (no. 114)	$P\bar{4}2_1c$ (no. 114)
a [Å]	9.38	13.22	13.29	9.380	9.3027(3)	9.2759(8)	9.38
b [Å]	9.38	13.49	13.49	9.380	9.3027(3)	9.2759(8)	9.38
c [Å]	6.71	6.83	6.83	6.700	6.6403(2)	6.6127(4)	6.70
α [°]	90	90	90	90	90	90	90
β [°]	90	90	90	90	90	90	90
γ [°]	90	90	90	90	90	90	90
V [Å ³]	590.375		1,224.5	589.495	574.65(3)	568.97	
Z	2	4	4	2	2	2	2
ρ_{calc} [g cm ⁻³]	1.778	1.716	1.715	1.781	1.827	1.845	1.773
T [K]	295	136 °C	295	295	123	100	

PETN has two common polymorphs: (i) PETN-I (tetragonal, stable up to 130 °C, mpt. = 142.9 °C) and (ii) PETN-II (orthorhombic, stable from 130 °C to its mpt. (143.1 °C))^[44]. PETN-II rapidly transforms to PETN-I at $T < 130$ °C. Impurities in PETN-II can inhibit transformation to the stable PETN-I^[44].

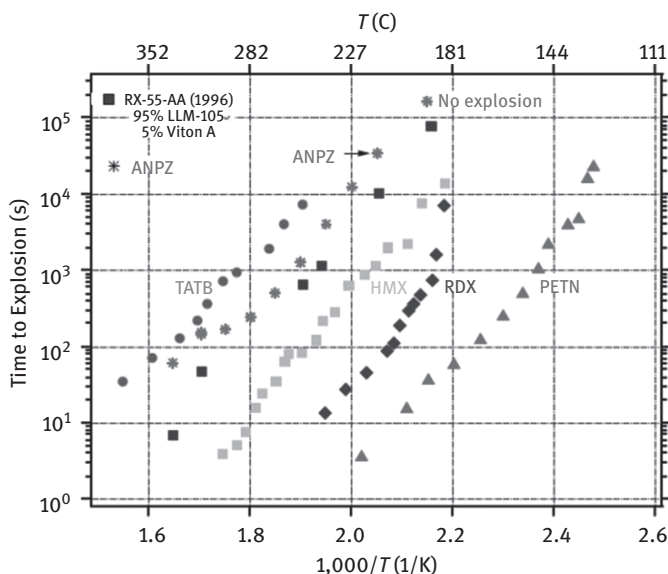
Pressure dependence of the volume of PETN @ 298 K^[87]:

Pressure (GPa)	Vol (Å ³) (approx. exptl. values, <i>Ohlinger</i>)	Vol (Å ³) (approx. exptl. values, <i>Ciezaketal</i>)	Vol (Å ³) (calcd. approx. values, PW91, VASP program package)
0	422	402	482
1	–	379	–
1.2	385	–	418
1.5	–	365	–
2.3	375	–	390
2.35	–	350	–
3.55	355	–	377
5.0	350	–	365
5.45	–	340	–
5.7	340	–	365
6.8	335	335	355
7.6	330	330	345
8.4	320	320	340
9.2	318	318	338
10.5	318	–	338

Failure diameters of lead and booster explosives^[119]:

Confinement, in			
Fabric detonating cord	Aluminum (0.006 walls)	Lead (MDF)	Heavy brass or steel
0.05	<0.05	<0.01	<0.05

Fig. 17 data from Ref. [120]

Fig. 17: ODTX results of ANPZ and TATB, HMX, RDX and PETN^[120].

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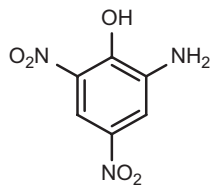
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Picramic acid

Name [German, acronym]: Picramic acid, dinitroaminophenol, 1,6-amino-2,4-dinitrophenol, 2-amino-4,6-dinitrophenol, 4,6-dinitro-2-aminophenol

Main (potential) use: No current applications and is a source for DDNP^[7]

Structural formula:



	Picramic acid	
Formula	C ₆ H ₅ N ₃ O ₅	
Molecular mass [g mol ⁻¹]	199.12	
Appearance at RT	Dark red crystals ^[7] , dark red needles from EtOH and prisms from CHCl ₃ ^[9]	
IS [J]	34 Nm ^[5]	
FS [N]	>353 ^[5]	
N [%]	21.10	
Ω(CO ₂) [%]	-76.3	
T _{m.p.} [°C]	168–169 ^[1] , 169.9 ^[5] , 169–170 ^[7, 9]	
T _{dec.} [°C]	240	
ρ [g cm ⁻³]	1.749 (@ 293 K) ^[2] , 1.685 (crystal @ 293 K) ^[6]	
Heat of formation	-1,248 kJ/kg (enthalpy of form.) ^[5] , -248.1 kJ/mol (enthalpy of form., exptl.) ^[10] , -201.8 kJ/mol (enthalpy of form., calcd., emp.) ^[10] , -229.9 kJ/mol (enthalpy of form., calcd., S-D method) ^[10]	
	Calcd. (EXPLO5 6.03)	Exptl.
-Δ _{ex} U° [kJ kg ⁻¹]	3,422	2,674 [H ₂ O (l)] ^[3, 5]
T _{ex} [K]	2,574	
p _{CJ} [kbar]	185	
VoD [m s ⁻¹]	6,938 (@ TMD)	
V ₀ [L kg ⁻¹]	636	847 ^[4, 5]

Trauzl test [cm ³ , % TNT]	166 cm ³ [8]
Burn rate [mm/s]	Ignites and burns rapidly in contact with open flame in glass tube or beaker ^[9]
Solubility [g/mL]	Soluble in benzene, acetic acid ^[7] , poorly soluble in other common organic solvents ^[7] , 0.065 g dissolves in 100 mL H ₂ O and only slightly more in hot water ^[9] , sparingly soluble in Et ₂ O, CHCl ₃ ^[9] , moderately soluble in EtOH ^[9] , soluble in benzene, glacial acetic acid, aniline ^[9]
Compatibility	Ignites and burns rapidly in contact with open flame in glass tube or beaker ^[9]
Flash point [°C]	Flashes @ 210 ^o [9]

	Picramic acid ^[6]
Chemical formula	C ₆ H ₅ N ₃ O ₅
Molecular weight [g mol ⁻¹]	199.12
Crystal system	Triclinic
Space group	<i>P</i> -1 (no. 2)
<i>a</i> [Å]	7.890(1)
<i>b</i> [Å]	8.174(1)
<i>c</i> [Å]	13.886(3)
α [°]	83.94(2)
β [°]	74.02(2)
γ [°]	65.76(2)
<i>V</i> [Å ³]	785.0(2)
<i>Z</i>	4
ρ_{calc} [g cm ⁻³]	1.685
<i>T</i> [K]	293

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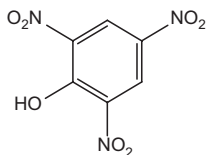
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Picric acid

Name [German, acronym]: 2,4,6-Trinitrophenol, melinite^[36], lyddite^[36, 48], pertite^[36], shimose^[36], picronitric acid, carbazotic acid, nitroxanthic acid [pikrinsäure, ekrasit (Austria)^[37], sprengkörper 88^[37], grf 88^[48], granatfullung 88^[48], bittersäure^[50], füllpulver Nr 2,5 & 24^[50], PA]

Main (potential) use: Secondary (high) explosive, explosive admixture, used in the manufacture of explosive D, main charge or booster explosive^[48]

Structural formula:



	PA
Formula	C ₆ H ₃ N ₃ O ₇
Molecular mass [g mol ⁻¹]	229.10
Appearance at RT	Pale yellow, flat needles if recryst. from H ₂ O (pure PA) ^[36] , colorless or yellow needles or lamellae ^[37] , lemon yellow crystalline powder but can vary in color from cream to yellow red ^[48] , yellow orthorhombic crystals obtained from EtOH ^[50] , light-bright yellow solid ^[9] , bright yellow crystalline substance which exists in two polymorphic forms ^[55] , aqueous solns. are yellow ^[55] , PA dissolved in sulfuric acid or ligroin produces colorless solns. ^[55] , yellow crystals (industrial PA) ^[55] , virtually colorless crystals if PA recryst. from sulfuric acid or hydrochloric acid ^[55] , pale yellow, odorless, intensely bitter crystals ^[61]
IS [J]	>50 ^[12] , 16.68 (85 cm, 2 kg mass, 20 mg sample, B.M.) ^[9, 10, 13] , 6.48 (13 in, 2 kg mass, 17 mg sample, P.A.) ^[9, 10, 13] , 16.0 ^[18] , $H_{50\%} = 65-93$ cm (B.M.) ^[19] , 13 in (P.A.) ^[19] , 9.5×10^3 kg/cm ² (critical stress for impact initiation) ^[19] , max. fall for $0/6$ shots >60 cm (2 kg mass, Lenze-Kast apparatus) ^[19] , max. fall for $0/6$ shots >24 cm (10 kg mass, Lenze-Kast apparatus) ^[19] , min. fall for $6/6$ shots >60 cm (2 kg mass, Lenze-Kast apparatus) ^[19] , min. fall for $6/6$ shots >24 cm (10 kg mass, Lenze-Kast apparatus) ^[19] , $H_{50\%} = 87$ cm ^[26, 35] , rel. scale = less sensitive than TNT ^[19] , 85 cm (2 kg mass, B.M.) ^[27] , $H_{50\%} = 64$ cm (B.M., type 12 tool, 2.5 kg mass, 35 mg sample, garnet paper) ^[28] , $H_{50\%} = 65$ cm (5 kg mass, PA contained in small 0.2 mm thick iron cup, covered with 0.2 mm thick small iron disc) ^[36] , $H_{50\%} = 30$ cm (5 kg mass) ^[36] , 87 cm (Bruceton method, type 12 tool, 2.5 kg mass, 40 mg sample, 5/0 sandpaper, 25 trials) ^[40] , $\log(H_{50}) = 1.940$ (Kamlet/Adolph) ^[45] , 42.5 cm (0 explosions in 5 trials, 2,000 g mass, BM small impact device) ^[49] , $H_{50\%} = 90$ cm (2.5 kg mass, type 12 tool, ERL method) ^[53] , 80 cm (2 kg mass) ^[55] , 13 in (17 mg sample, P.A.) ^[56] , 100+ cm (B.M.) ^[56] , $H_{50\%} = 64$ cm (2.5 kg mass) ^[64]

FS [N]	>363 ^[10] , explodes if powder is exposed to friction between plates of iron, steel or stones ^[55] , wood mallet on stone = 0% ^[58] , wood mallet on soft wood = 0% ^[58] , wood mallet on hard wood = 0% ^[58]																		
ESD [J]	8.98 ^[5, 18, 65]																		
N [%]	18.34																		
Ω(CO ₂) [%]	−45.39																		
T _{m.p.} [°C]	122 ^[1, 13, 19, 27, 48, 56] , 124 ^[20] , 121.8–122.4 ^[29] , 122.5 ^[36, 37, 50, 58] , (setting point = 121.3 ^[37] , sublimes > mpt. ^[37]), 121.8–122.4 (Thomas Hoover capillary melting point apparatus @ 2 °C/min) ^[42] , 123 ^[46] , 121.8 ^[52] , 122–123 ^[9, 61] , 122.5 (orthorhombic crystals) ^[55] , 121.3 (freezing point, orthorhombic crystals) ^[55]																		
T _{b.p.} [°C]	195 (@ 2 mm Hg) ^[39] , 255 (@ 50 mm Hg) ^[39] , 325 ± 10 (@ 760 mm Hg, most probable value) ^[39] , 160–198 ^[43]																		
T _{dec.} [°C]	237 (DSC @ 5 °C/min), >300 (DSC @ 5 °C/min) ^[1] , 190 (77%, DSC) ^[12] , 332 (exotherm peak max., DSC @ 20 °C/min) ^[20] , 160 (slight dec.) ^[37]																		
ρ [g cm ^{−3}]	<p>1.822 (@ 120 K), 1.748 (@ 298 K, gas pycnometer), 1.77 (@ 293 K, gas pycnometer)^[2], 1.76 (crystal)^[13, 27], 1.76^[19, 46, 60], 1.763^[61]</p> <p>Loading ρ @ different pressures:</p> <table><tr><th>Pressure (kpsi)</th><th>ρ (g cm^{−3})</th></tr><tr><td>3</td><td>1.4^[13, 27, 56]</td></tr><tr><td>5</td><td>1.5^[13, 27, 56]</td></tr><tr><td>10</td><td>1.57^[13, 27, 56]</td></tr><tr><td>12</td><td>1.59^[13, 27, 56]</td></tr><tr><td>15</td><td>1.61^[13, 27, 56]</td></tr><tr><td>20</td><td>1.64^[13, 27, 56]</td></tr><tr><td>Cast</td><td>1.71^[27, 56]</td></tr><tr><td>Crystal</td><td>1.76^[27, 56]</td></tr></table> <p>1.767^[35, 45], sp. gr. = 1.813^[37], sp. gr. = 1.589 (molten PA @ 124 °C)^[37, 55], sp. gr. = 1.513 (molten PA @ 170 °C)^[37], apparent weight of crystal. PA = 0.9–1.0^[37], 1.763 (crystal)^[50], 1.64 (pressed @ 20,000 psi)^[50], 1.71 (cast)^[50], sp. gr. = 1.763 (crystalline)^[55], 0.9–1.0 (gravimetric density)^[55], 1.61–1.67 (cast)^[55], 1.63 (pressed @ 2,000 kg/cm²)^[55], 1.74 (pressed @ 4,125 kg/cm²)^[55], 1.81^[58]</p>	Pressure (kpsi)	ρ (g cm ^{−3})	3	1.4 ^[13, 27, 56]	5	1.5 ^[13, 27, 56]	10	1.57 ^[13, 27, 56]	12	1.59 ^[13, 27, 56]	15	1.61 ^[13, 27, 56]	20	1.64 ^[13, 27, 56]	Cast	1.71 ^[27, 56]	Crystal	1.76 ^[27, 56]
Pressure (kpsi)	ρ (g cm ^{−3})																		
3	1.4 ^[13, 27, 56]																		
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15	1.61 ^[13, 27, 56]																		
20	1.64 ^[13, 27, 56]																		
Cast	1.71 ^[27, 56]																		
Crystal	1.76 ^[27, 56]																		

	<p>ρ of PA depending on the pressure applied, values from^[37]:</p> <table> <tr> <th>Pressure applied (kg/cm²)</th><th>Average ρ (g cm⁻³)</th><th>Pressure Applied (kg/cm²)</th><th>Average ρ (g cm⁻³)</th></tr> <tr> <td>275</td><td>1.315</td><td>2,750</td><td>1.714</td></tr> <tr> <td>685</td><td>1.480</td><td>3,435</td><td>1.731</td></tr> <tr> <td>1,375</td><td>1.614</td><td>4,125</td><td>1.740</td></tr> <tr> <td>2,060</td><td>1.672</td><td></td><td></td></tr> </table> <p>1.63 (@ 4,000 kg/cm², <i>Kast</i>)^[37], 1.74 (@ 4,500 kg/cm²)^[37], 1.66 (solidified PA on slowly cooling molten PA)^[37], 1.70 (solidified PA on rapidly cooling molten PA)^[37]</p>			Pressure applied (kg/cm ²)	Average ρ (g cm ⁻³)	Pressure Applied (kg/cm ²)	Average ρ (g cm ⁻³)	275	1.315	2,750	1.714	685	1.480	3,435	1.731	1,375	1.614	4,125	1.740	2,060	1.672		
Pressure applied (kg/cm ²)	Average ρ (g cm ⁻³)	Pressure Applied (kg/cm ²)	Average ρ (g cm ⁻³)																				
275	1.315	2,750	1.714																				
685	1.480	3,435	1.731																				
1,375	1.614	4,125	1.740																				
2,060	1.672																						
Heat of formation	<p>−51.3 kcal mol⁻¹ (standard heat of form.)^[19], −217.9 kJ/mol^[11], −213.6 kJ/mol^[2], −51.3 kcal/mol^[14], −248.53 kJ/mol (enthalpy of form.)^[43], 63.3 kcal/mol (ΔH_f)^[37], −46.8–50.9 kcal/mol (ΔH_f)^[37], −226.0 kcal/kg (enthalpy of form.)^[41], 208.9 kcal/kg^[54], −52.07 kcal/mol ($\Delta_f H$ (s))^[35], 248 kcal/kg^[13, 30], −214.5 kJ/mol (ΔH_f)^[60], 59.40 kcal/mol (−ΔH_f (heat of form. @ standard conditions))^[63]</p>																						
Heat of combustion	<p>2,672 kcal/kg^[13, 30, 56], 2,696 kcal/kg (@ C^V)^[54], $\Delta H_c = 621.2$ kcal/mol (@ C^V)^[37], heat of comb. = 611.93 kcal/mol (@ 1 atm.)^[62]</p> <p>Exptl. heat of combustion data^[63]:</p> <table> <tr> <th>−$\Delta U_{B/M}$ (cal/g)</th><th>−ΔU_B (kcal/mol)</th><th>−ΔU_R (kcal/mol @ 1 atm. and constant vol.)</th><th>−ΔH_R (kcal/mol @ 1 atm. and constant pressure)</th></tr> <tr> <td>2,687.21 ± 0.84</td><td>615.69</td><td>614.44</td><td>611.93</td></tr> </table>			− $\Delta U_{B/M}$ (cal/g)	− ΔU_B (kcal/mol)	− ΔU_R (kcal/mol @ 1 atm. and constant vol.)	− ΔH_R (kcal/mol @ 1 atm. and constant pressure)	2,687.21 ± 0.84	615.69	614.44	611.93												
− $\Delta U_{B/M}$ (cal/g)	− ΔU_B (kcal/mol)	− ΔU_R (kcal/mol @ 1 atm. and constant vol.)	− ΔH_R (kcal/mol @ 1 atm. and constant pressure)																				
2,687.21 ± 0.84	615.69	614.44	611.93																				
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.																				
− $\Delta_{ex} U^o$ [kJ kg ⁻¹]	4,604	<p>4,184^[4]</p> <p>1,000 kcal/kg^[30]</p> <p>1.2 kcal/g (@ 1.76 g cm⁻³, calcd., <i>Mader</i>)^[19]</p> <p>1.02 kcal/g (@ 1.00 g cm⁻³, calcd., <i>Mader</i>)^[19]</p> <p>1.28 kcal/g (Q_{max}, calcd.)^[35]</p> <p>910–935 kcal/kg^[37]</p>	<p>3,437 [H₂O (l)]^[8]</p> <p>1,000 cal/g^[13, 56]</p> <p>1,010 kcal/kg [H₂O (g)]^[17]</p> <p>1,010 kcal/kg (@ 1.700 g cm⁻³) [H₂O vapor]^[41]</p> <p>1,050 kcal/kg^[55]</p>																				

		1,000 kcal/kg (<i>Kast</i>) ^[37] 960 kcal/kg (<i>Schmidt</i>) ^[37] 810 cal ^[39] 1,054 kcal/kg (@ 1.700 g cm ⁻³ , calcd.) [H ₂ O vapor] ^[41] $-\Delta H_{\text{det}} = 3.59 \text{ kJ/g}$ ^[60]	
T_{ex} [K]	3,484	3,230 (no units given, probably °C) ^[4, 30] 3,230 °C (<i>Kast</i>) ^[37] 3,530 °C (<i>Schmidt</i>) ^[37] 2,430 °C ^[39] 3,280 (@ 1.76 g cm ⁻³ , calcd. BKWR) ^[14] 3,330 (@ 1.71 g cm ⁻³ , calcd. BKWR) ^[14] 3,420 (@ 1.60 g cm ⁻³ , calcd. BKWR) ^[14] 4,010 (@ 1.76 g cm ⁻³ , calcd. BKWS) ^[14] 4,030 (@ 1.71 g cm ⁻³ , calcd. BKWS) ^[14] 4,080 (@ 1.60 g cm ⁻³ , calcd. BKWS) ^[14]	3,300–3,500 °C ^[55]
$p_{\text{C-I}}$ [kbar]	234	251 (@ 1.767 g cm ⁻³ , calcd.) ^[35] 259 (@ 1.76 g cm ⁻³ , calcd. BKWR) ^[14] 243 (@ 1.71 g cm ⁻³ , calcd. BKWR) ^[14] 210 (@ 1.60 g cm ⁻³ , calcd. BKWR) ^[14] 237 (@ 1.76 g cm ⁻³ , calcd. BKWS) ^[14]	2,150 kg/cm ² (@ 0.20 g cm ⁻³ , piston and obturator) ^[36] 3,055 kg/cm ² (@ 0.25 g cm ⁻³ , piston and obturator) ^[36] 3,865 kg/cm ² (@ 0.30 g cm ⁻³ , piston and obturator) ^[36] 0.187 Mbar ^[56]

		222 (@ 1.71 g cm ⁻³ , calcd. BKWS) ^[14] 192 (@ 1.60 g cm ⁻³ , calcd. BKWS) ^[14]	
VoD [m s ⁻¹]	7,472	7,100 (@ 1.69 g cm ⁻³) ^[4] 7,460 (@ 1.70 g cm ⁻³) ^[31] 7,100 (@ 1.59–1.70 g cm ⁻³ , av. value from lit.) ^[31] 7,200 (@ 1.7 g cm ⁻³) ^[30] 7,680 (@ 1.76 g cm ⁻³ , calcd., <i>Mader</i>) ^[19] 5,545 (@ 1.00 g cm ⁻³ , calcd., <i>Mader</i>) ^[19] 7,360 (@ 1.76 g cm ⁻³ (TMD), calcd., R-P method) ^[33] 7,570 (@ 1.767 g cm ⁻³ , calcd.) ^[35] 7,580 (@ 1.76 g cm ⁻³ (TMD), calcd., <i>Aizenshtadt</i>) ^[33] 7,510 (@ 1.76 g cm ⁻³ (TMD), calcd., K-J) ^[33] 7,360 (@ 1.76 g cm ⁻³ (TMD), calcd., R-P method) ^[33] 7,100–7,150 generally accepted as highest VoD values found ^[37] 7,510 (@ 1.76 g cm ⁻³ , calcd. BKWR) ^[14] 7,360 (@ 1.71 g cm ⁻³ , calcd. BKWR) ^[14] 7,030 (@ 1.60 g cm ⁻³ , calcd. BKWR) ^[14] 7,520 (@ 1.76 g cm ⁻³ , calcd. BKWS) ^[14]	5,270 (@ 1.64 g cm ⁻³ , pressed, 1.0 in charge diameter) ^[13] 7,350 (@ 1.71 g cm ⁻³ , cast, 1.25 in charge diameter) ^[13] 7,570 (@ 1.76 g cm ⁻³) ^[6, 7, 8, 14] 7,260 (@ 1.71 g cm ⁻³) ^[6, 8, 14, 34] 7,260 (@ 1.7 g cm ⁻³) ^[37] 7,100 (@ 1.60 g cm ⁻³) ^[6, 8, 14] 5,210 (@ 1.64 g cm ⁻³ , pressed) ^[9] 7,390 (@ 1.71 g cm ⁻³ , cast) ^[9] 7,350 (@ 1.70 g cm ⁻³) ^[16] 4,965 (@ 0.97 g cm ⁻³) ^[19] 6,190 (@ 1.32 g cm ⁻³) ^[19] 6,510 (@ 1.41 g cm ⁻³) ^[19] 7,200 (@ 1.62 g cm ⁻³) ^[19] 7,480 (@ 1.70 g cm ⁻³) ^[19] 7,160 (@ 1.6 g cm ⁻³) ^[30] 7,350 (cast) ^[27] 6,777 (cast PA) ^[36] 4,835 (@ 0.862 g cm ⁻³ , compressed PA) ^[36] 4,970 (@ 0.98 g cm ⁻³ , extra light Pb tubing) ^[39] 5,980 (@ 1.30 g cm ⁻³ , unconfined charge of 21 mm diameter, 1 g detonator) ^[37]

		<p>7,350 (@ 1.71 g cm⁻³, calcd. BKWS)^[14]</p> <p>6,970 (@ 1.60 g cm⁻³, calcd. BKWS)^[14]</p>	<p>6,465 (@ 1.41 g cm⁻³, unconfined charge of 21 mm diameter, 1 g detonator)^[37]</p> <p>6,885 (@ 1.49 g cm⁻³, unconfined charge of 21 mm diameter, 1 g detonator)^[37]</p> <p>7,110 (@ 1.50 g cm⁻³, unconfined charge of 21 mm diameter, 1 g detonator)^[37]</p> <p>4,020 (@ 0.70 g cm⁻³, metal pipe, 10–15 mm diameter)^[37]</p> <p>4,635 (@ 0.90 g cm⁻³, metal pipe, 10–15 mm diameter)^[37]</p> <p>6,190 (@ 1.30 g cm⁻³, metal pipe, 10–15 mm diameter)^[37]</p> <p>6,930 (@ 1.54 g cm⁻³, metal pipe, 10–15 mm diameter)^[37]</p> <p>4,560 (@ 1.1 g cm⁻³, bakelite pipe, 4.5–8.2 mm diameter)^[37]</p> <p>5,430 (@ 1.23 g cm⁻³, bakelite pipe, 4.5–8.2 mm diameter)^[37]</p> <p>6,940 (@ 1.41 g cm⁻³, bakelite pipe, 4.5–8.2 mm diameter)^[37]</p> <p>7,504 (@ 1.56 g cm⁻³, bakelite pipe, 4.5–8.2 mm diameter)^[37]</p> <p>23,200 ft/s (@ 1.6 /mL)^[48]</p> <p>7,350 (@ 1.71 g cm⁻³ (cast ρ))^[50]</p> <p>5,270 (@ 1.64 g cm⁻³, pressed)^[9]</p> <p>7,390 (@ 1.71 g cm⁻³, cast)^[9]</p> <p>6,800 (@ 1.59 g cm⁻³)^[58]</p> <p>7,080 (@ 1.60 g cm⁻³)^[62]</p>
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V_0 [L kg ⁻¹]	638	675 (@ 0 °C) ^[4] 725 (<i>Robertson, Garner</i>) ^[37] 737 (<i>Schmidt</i>) ^[37] 675 (<i>Kast</i>) ^[37] 877 (@ 0 °C and 760 mm Hg) ^[39]	675 ^[13] 826 ^[15] 730 ^[55]
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VoD values (m/s) in cylindrical charges of 3.17 cm diameter, unconfined, cast PA, $\rho=1.71$ g cm⁻³, no. shots fired = 10^[51]: 7,296, 7,275, 7,275, 7,274, 7,273, 7,263, 7,257, 7,239, 7,235, 7,227, mean value = 7,260 m/s^[51]

Critical T [K]	903 (explosion in 250 μ s) ^[53]
Trauzl test [cm ³ , % TNT]	101% TNT ^[9, 13, 19] , 103–117% TNT ^[31] , 30–365 cc (10 g charge) ^[27] , 250–350 mL ^[37] , 12.4 cc (small Trauzl test) ^[39, 49] , 470 cc (15 g sample) ^[36] , 300 cm ³ (sand tamping, 10 g sample) ^[39] , more powerful than TNT ^[50] , 305 cc ^[55] , 315 ^[59] , 332 ^[59]
Small lead block compression test	50 g PA, exploded by detonator on top of 64 mm long lead cylinder = 16.4 mm block shortening ^[39] , PA detonated by detonator containing 1.5 g fulminate, 40 g exploded on 67 mm diameter Pb block produced shortening of 10.5 mm ^[39]
Sand test [g]	48.5 g (200 g bomb) ^[9, 13] , 103–110% TNT ^[31] , 113% TNT ^[27] , 41.8 g sand crushed (1,700 g bomb, 0.4 g sample) ^[31] , 104% TNT ^[37] , 57.0 g (amount of sand crushed finer than 30 mesh, by total charge consisting of base charge of 0.50 g PA and 0.30 g priming charge of MF) ^[49] , 45.3 g (amount of sand crushed finer than 30 mesh, by base charge of 0.50 g PA) ^[49] , rel. strength cf. TNT = 1.04 ^[49]
Ballistic mortar test	112% TNT ^[9, 13, 19, 62] , 106–112% TNT ^[31] , 110–120% TNT ^[37]
Ballistic pendulum test	More powerful than TNT ^[50]
Initiating efficiency	Minimum initiating charge of primary explosive (g) required to initiate explosion in 0.5 g PA in a No. 8 detonator shell, both explosives compressed under 3,400 lb/in ² ^[39] : 0.115 g DDNP ^[39] , 0.225 g MF ^[39] , 0.12 g LA ^[39] , 0.24 g minimum detonating charge LA ^[56] Minimum amount of primary explosive (g) needed to cause detonation of PA ^[39] : 0.02 g cadmium azide ^[39] , 0.035 g SA ^[39] , 0.025 g LA ^[39] , 0.045 cuprous azide ^[39] , 0.075 g mercurous azide ^[39] , 0.115 g thallium azide ^[39] , 0.005 g silver fulminate ^[39] , 0.05 g cadmium fulminate ^[39] , 0.08 g copper fulminate ^[39] , 0.30 g MF ^[39] , 0.43 g thallium fulminate ^[39]

	<p>Minimum initiating charge (g) required for 0.4 g PA in detonator capsule, initiator added, pressed down, short reinforcing cap, pressed @ 200 atm/in²^[39]: 0.05 g cyanuric azide^[39], 0.21 g MF^[39]</p> <p>Minimum initiating charge (g) required for 0.4 g PA, compressed in detonator capsule, pressed @ 1,000 lb/in²^[39]: 0.21 g fulminate (with reinforcing cap)^[39], 0.05 g HMTD (with reinforcing cap)^[39], 0.06 g HMTD (without reinforcing cap)^[39]</p> <p>Minimum weight of priming charge which causes complete detonation of the base charge^[49]: 0.115 g DDNP^[49], 0.225 g MF^[49], 0.12 g LA^[49]</p>																								
5 s explosion <i>T</i> [°C] 5 s ignition <i>T</i> [°C]	295–310 ^[30] , 320 (dec.) ^[13] , 320 (dec., cook off) ^[56] 322 ^[19] , 320 (dec.) ^[30] , 320 (dec., USA value) ^[30] , 295–322 (dec., Russian value) ^[30]																								
Explosion <i>T</i> [°C]	300–310 (slow heating, heating rate @ 20 °C/min) ^[19] , 316 (bath heating rate 20 °C/min) ^[19] , 309 (bath heating rate 5 °C/min) ^[19] , 260 °C (30 min) ^[37] , >300–310 (explosion, if rapidly heated) ^[37] , 320 ^[50] , 300 (rapid heating in an enclosed shell) ^[55] , explodes above 300 ^o ^[61] , explodes when rapidly heated ^[61]																								
Initiation <i>T</i> [°C] Ignition <i>T</i> [°C]	243–288 (slow heating) ^[37] , 337–346 (rapid heating) ^[37] 300–310 (vacuum) ^[39] , 316 (heated from 100 °C @ 20 °C/min) ^[36] , 309 (heated from 100 °C @ 5 °C/min) ^[36]																								
Detonating <i>T</i> [°C]	<p><i>T</i> (°C) and time to explosion (s), 25 mg sample^[47]:</p> <table><tr><td><i>T</i> (°C)</td><td>Time (s)</td><td><i>T</i> (°C)</td><td>Time (s)</td></tr><tr><td>350</td><td>1.48</td><td>277</td><td>26.3</td></tr><tr><td>330</td><td>2.96</td><td>273</td><td>29.6</td></tr><tr><td>312</td><td>5.50</td><td>267</td><td>50.3</td></tr><tr><td>294</td><td>11.8</td><td>260</td><td>No explosion</td></tr><tr><td>286</td><td>16.6</td><td></td><td></td></tr></table> <p>~320^[48], 320 (5 s)^[9], 300–310 (deflagration)^[55]</p>	<i>T</i> (°C)	Time (s)	<i>T</i> (°C)	Time (s)	350	1.48	277	26.3	330	2.96	273	29.6	312	5.50	267	50.3	294	11.8	260	No explosion	286	16.6		
<i>T</i> (°C)	Time (s)	<i>T</i> (°C)	Time (s)																						
350	1.48	277	26.3																						
330	2.96	273	29.6																						
312	5.50	267	50.3																						
294	11.8	260	No explosion																						
286	16.6																								
Thermal stability	<p><i>T</i> (°C)/ time to explosion (s) (25 mg samples, small diameter thin-walled Cu tubes)^[19, 32]: 350/1.5, 315/5.5, 277/26.3, 267/50.3, 260/failed^[19, 32]</p> <p>Ignition <i>T</i> (°C)/heating times (min) after bath reached 100 °C^[27]: 243/13.25 (ignition), 281/17.17 (ignition), 281/19.25 (ignition), 262/36.47 (ignition)^[27]</p> <p>No. of moles gas produced per mole PA/no. h^[20]: 0/22 (@ 120 °C)^[20], 0/72 (@ 120 °C)^[20], 3.47/22 (@ 220 °C)^[20], 3.64/72 (@ 220 °C)^[20], 3.89/22 (@ 320 °C)^[20], 4.09/72 (@ 320 °C)^[20]</p> <p>Long-term storage tests at normal temperatures shows no measurable deterioration^[9, 50], 2.8 cc/g/h @ 210 °C^[53], stable at usual storage temperatures^[55], explodes when rapidly heated^[61]</p>																								

100 °C heat test [% mass loss]	0.03% loss in first 48 h ^[13] , 0.09% loss in second 48 h ^[13] , no explosion in 100 h ^[13]																																						
75 °C Int. heat test	0.05% loss in 48 h ^[13]																																						
Vacuum stability test [cm ³ /h]	0.2 cc/40 h @ 100 °C ^[13] , 0.5 cc/40 h @ 120 °C ^[13, 56]																																						
Vapor pressure [atm. @ °C]	2 mm Hg @ 195 °C ^[13, 19] , 50 mm Hg @ 255 °C ^[13, 19] , 7.47×10^{-7} Torr @ 25 °C ^[46] , 7.5×10^{-7} mm Hg @ 25 °C ^[52] , 2 mm Hg @ 195 °C ^[55] , 50 mm Hg @ 225 °C ^[55]																																						
Burn rate [mm/s]	<p>Large quantities have been burned without explosion but explosion risk remains^[48], ignited PA burns slowly with a smoky flame in open air or wood packaging^[55]</p> <p>Mass burn rate of volatile explosives^[57]:</p> <table><tr><th colspan="5">$m, \text{ gm cm}^{-2} \text{ s}^{-1}$</th></tr><tr><td>40 atm</td><td>100 atm</td><td>200 atm</td><td>400 atm</td><td>1,000 atm</td></tr><tr><td>0.46</td><td>0.945</td><td>1.75</td><td>3.36</td><td>8.19</td></tr></table> <p>Burn rate and equilibrium combustion temperature^[57]: $T_e = 2,475 \text{ K}^{[57]}$, $m = 0.945 \text{ g cm}^{-2} \text{ s}^{-1}$ (100 atm.)^[57]</p> <p>Dependence of burning rate of volatile explosives on pressure, PA $\rho_{\text{max}} = 1.81 \text{ g/cm}^3$^[57]:</p> <table><tr><th rowspan="2">$\delta = \rho/\rho_{\text{max}}$</th><th colspan="3">Coefficients in formulae</th><th rowspan="2">Pressure, atm.</th></tr><tr><th>a</th><th>b</th><th>N</th></tr><tr><td>~1.0</td><td>0.14</td><td>0.008</td><td>1.0</td><td>25–950</td></tr><tr><td></td><td>–</td><td>0.036</td><td>0.68</td><td>25–80</td></tr><tr><td></td><td>–</td><td>0.0101</td><td>0.97</td><td>80–950</td></tr></table>	$m, \text{ gm cm}^{-2} \text{ s}^{-1}$					40 atm	100 atm	200 atm	400 atm	1,000 atm	0.46	0.945	1.75	3.36	8.19	$\delta = \rho/\rho_{\text{max}}$	Coefficients in formulae			Pressure, atm.	a	b	N	~1.0	0.14	0.008	1.0	25–950		–	0.036	0.68	25–80		–	0.0101	0.97	80–950
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Solubility [g/mL]	Solubility (g/100 solvent, %) ^[13] :									
	Water		Alcohol		Benzene		Toluene		Ether	
	°C	%	°C	%	°C	%	°C	%	°C	%
	0	0.85	0	4.5	0 ~ 2	20 ~ 13	20 ~			
	20	1.17	20	6.9	20	9.6	60 ~ 30	34.7	3.96	
	40	1.88	40	12.0	40	27.5				
	60	2.98			60	59				
	80	4.53								
	100	7.1								
	Chloroform		Ethyl acetate		Carbon tetrachloride		Pyridine		Acetone	
	°C	%	°C	%	°C	%	°C	%	°C	%
	20 ~ 2	20	42	20 ~ 0.07	10	24	20	125		
	60 ~ 6	30	50	60 ~ 0.4	30	37.5	30	137		
			40	58			50	58	40	164
			50	69					50	208
	MeOH		Isopropyl alcohol		Propanol-1		Carbon disulfide			
	°C	%	°C	%	°C	%	°C	%		
	0	14	10	6.4	0	2.4	20	0.12		
	20	19	30	9.8	20	3.3	30	0.16		
	40	31	50	15.5	40	5.4				
	50	41			50	7.4				

Solubility in H₂O^[37]:

T (°C)	Amount of PA (g) dissolved in 100 g H ₂ O	T (°C)	Amount of PA (g) dissolved in 100 g H ₂ O
0	0.68	60	2.81
10	0.81	70	3.47
20	1.11	80	4.41
30	1.40	90	5.72
40	1.78	100	7.24
50	2.19		

Solubility in organic solvents^[37]:

Solvent	T (°C)	Amount of solvent (parts)	Amount of PA (parts)
EtOH	25	100	7.452
Et ₂ O	13	100	1.08
Et ₂ O (H ₂ O saturated)	13	100	4.00
Benzene	6	100	3.50
Benzene	15	100	5.9
Toluene	20	100 mL soln.	12.0 g
Amyl alcohol	20	100 mL soln.	1.755 g

Solubility in aqueous solns. of alcohols and acetone^[37]:

% of organic component of soln.	Amount of PA (g) dissolved in 100 g @ 25 °C		
	MeOH	EtOH	Acetone
0	1.3	1.3	1.3
30	2.4	3.1	9.5
60	7.1	10.5	46.7
80	–	13.8	87.8
81	–	13.8	–
85	–	13.2	–
90	16.0	12.3	–
100	21.1	8.0	43

Aqueous solubility = 12,400 mg/L @ 25 °C^[46], slightly soluble in H₂O, Et₂O^[48], moderately soluble in EtOH, ⁱPrOH, and benzene^[48], soluble in toluene, MeOH and baking soda soln.^[48], very soluble in acetone^[48], slightly soluble in water at normal temperature^[50], moderately soluble in hot water^[50], slightly soluble in Et₂O, CCl₄ and CS₂^[50], readily soluble in hot EtOH, benzene, toluene, acetone, MeOH and other solvents^[50], 12,800 mg/L in H₂O @ 25 °C^[52]

Solubility data in water from^[55]:

<i>T</i> (°C)	Solubility of PA g/100 g solvent	<i>T</i> (°C)	Solubility of PA g/100 g solvent
0	1.05	40	1.98
5	1.07	50	2.53
10	1.10	60	3.17
15	1.16	70	3.89
20	1.22	80	4.66
25	1.37	90	5.49
30	1.55	100	6.33

Solubility in sulfuric acid data from^[55]:

Strength of sulfuric acid	Solubility, g PA/100 g acid @ <i>T</i> (°C)		
	18 °C	50 °C	80 °C
0	1.184	2.389	4.541
2.3	0.0230	0.692	1.940
4.7	0.142	0.368	1.251
10.0	0.091	0.265	0.727
18.0	0.049	0.214	0.561
25.5	0.092	0.230	0.587
50.5	0.429	0.645	1.104
69.7	0.928	1.424	2.203
87.9	2.451	5.826	7.610
97.4	7.532	12.785	24.024
100.0	10.180	16.230	25.860

Solubility data in organic solvents from^[55]:

Solvent	Solubility of PA, % at temperatures in °C											
	15	20	27	35	38	42	48	51	56	60	65	78
Alcohol	–	5.9										40
Dichlorobenzene	–	3.45								8.4		
Nitrobenzene	–	28.3		33.3		38.3		42.5	46.2			
Dichloroethane	9.1		12.3	14.3	16.7		22.7		29.4		39.7	
Benzene	6.8	8.8	11.4	17.6		23.5			33.5		41.7	50

Soluble in Et₂O, MeOH, glycerin, CHCl₃, CS₂ and in resins and lacquers^[55],

1 g dissolves in: 78 mL water^[61], 15 mL boiling water^[61], 12 mL EtOH^[61], 10 mL benzene^[61], 35 mL CHCl₃^[61], 65 mL Et₂O^[61]

Partition coefficients

Partition coefficients for PA between two liquid phases: either water–toluene or water–Et₂O^[37]:

Conc. of PA in soln. (g/L)	Soln. vols.	Amount of PA (g) dissolved in 100 mL soln.		Partition coefficient
	H ₂ O– Toluene	H ₂ O	Toluene	
10	100:100	0.275	0.725	1:2.63
3		0.125	0.175	1:1.24
1		0.062	0.038	1:0.63
0.1		0.010	–	–
-	H ₂ O–Et ₂ O	H ₂ O	Et ₂ O	–
10	106:96	0.374	0.670	1:1.79
1		0.085	0.011	1:0.129
0.1		0.0105	0.00011	1:0.010
0.01		0.000952	–	–

	Values from ^[37] , partition coefficient $k = C_1^n/C_2$; n = temperature-independent exponent, C_1 and C_2 = concentrations: <table><tr><th>T (°C)</th><th>Benzene–H₂O ($N = 1.727 \text{ k} \times 10^2$)</th><th>$T$ (°C)</th><th>Toluene–H₂O ($N = 1.677 \text{ k} \times 10^2$)</th><th>Chlorobenzene–H₂O ($N = 1.674 \text{ k} \times 10^2$)</th></tr><tr><td>10</td><td>1.563</td><td>20</td><td>1.875</td><td>2.421</td></tr><tr><td>30</td><td>1.892</td><td>40</td><td>2.323</td><td>2.965</td></tr><tr><td>50</td><td>2.275</td><td>60</td><td>2.884</td><td>3548</td></tr><tr><td>70</td><td>2.673</td><td>80</td><td>3.532</td><td>4.416</td></tr></table>	T (°C)	Benzene–H ₂ O ($N = 1.727 \text{ k} \times 10^2$)	T (°C)	Toluene–H ₂ O ($N = 1.677 \text{ k} \times 10^2$)	Chlorobenzene–H ₂ O ($N = 1.674 \text{ k} \times 10^2$)	10	1.563	20	1.875	2.421	30	1.892	40	2.323	2.965	50	2.275	60	2.884	3548	70	2.673	80	3.532	4.416
T (°C)	Benzene–H ₂ O ($N = 1.727 \text{ k} \times 10^2$)	T (°C)	Toluene–H ₂ O ($N = 1.677 \text{ k} \times 10^2$)	Chlorobenzene–H ₂ O ($N = 1.674 \text{ k} \times 10^2$)																						
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50	2.275	60	2.884	3548																						
70	2.673	80	3.532	4.416																						
Log K_{ow}	2.03 ^[46] , 1.33 ^[52]																									
Log K_{oc}	2.00 ^[46]																									
Hygroscopicity	0.04% @ 30 °C with 90% RH ^[13] , only slightly hygroscopic ^[37] , PA in contact with H ₂ O-saturated air @ 32 °C for 48 h absorbed 0.37% H ₂ O ^[37] , slightly hygroscopic ^[48] , nonhygroscopic ^[9] , virtually nonhygroscopic ^[55]																									
Radiation sensitivity	No drop in chemical stability after exposure to γ -rays with intensity of 3×10^4 Roentgens/h administering doses of 0.5–20 megaroentgens with total exposure times of 15–660 h (cobalt-60 source) ^[50]																									
Compatibility	Presence of moisture increases reactivity especially with metals ^[48] , reacts with all metals except Al and Sn ^[48] , is highly acidic and corrosive ^[48] , forms very dangerous mixtures with lead or lead compounds ^[48] , dry PA has little effect on ordinary metals ^[50] , moist PA in contact with Fe, Pb, Ni, Zn or Cu can form dangerous picrates ^[50] , molten PA can form picrates on contact with Pb or Zn ^[50] , PA reacts with all metals except Al and Sn ^[9] , incompatible with all oxidizable substances, albumin, gelatin and alkaloids ^[61]																									
Specific heat [cal/g]	Values from ^[13] : <table><tr><th>T(°C)</th><th>Specific heat (cal/g/°C)</th></tr><tr><td>0</td><td>0.235</td></tr><tr><td>30</td><td>0.258</td></tr><tr><td>60</td><td>0.282</td></tr><tr><td>90</td><td>0.310</td></tr><tr><td>120</td><td>0.337</td></tr></table>	T (°C)	Specific heat (cal/g/°C)	0	0.235	30	0.258	60	0.282	90	0.310	120	0.337													
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T (°C)	Specific heat (cal/g)	T (°C)	Specific heat (cal/g)																		
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20	0.250	100	0.318																		
40	0.266	120	0.337																		
60	0.282																				
Heat capacity [J•mol ⁻¹ •K ⁻¹]	$C^0_{p,m} = 211.13$ @ 298.15 K (calcd.) ^[66] , 258.59 @ 400.00 K (calcd.) ^[66] , 295.72 @ 500.00 K (calcd.) ^[66] , 324.47 @ 600.00 K (calcd.) ^[66] , 346.67 @ 700.00 K (calcd.) ^[66] , 363.99 @ 800.00 K (calcd.) ^[66]																				
Heat of solidification [cal/mol]	4.30 ^[37] , 4.66 ^[37]																				
Heat of fusion [cal/g]	20.4 ^[13] , 20 ^[46] , 20.4 (latent heat of fusion) ^[55]																				
ΔH_{sub} [kJ/mol]	105.1 (exptl.) ^[44] , 111.3 (calcd., QSPR) ^[44]																				
Diffusion coefficient [cm ² /s]	0.066 (air) ^[46] , 7.03×10^{-6} (water) ^[46]																				
Rifle bullet impact test	60% partials, 40% burned, 0% explosions, 0% unaffected in trials ^[13]																				
Plate dent test	Brisance = 107% TNT, method A, pressed, not confined, $\rho = 1.50$ g cm ⁻³ ^[13]																				
Booster sensitivity test	Pressed, 10 g tetryl, 2 g wax, $\rho = 1.6$ g cm ⁻³ ^[13] ; cast, 5 g tetryl, 0 g wax, $\rho = 1.7$ g cm ⁻³ ^[13] ; 50% detonation sensitivity, 100 g tetryl, 2 g wax gap, $\rho = 1.7$ g cm ⁻³ ^[56]																				
Thermal conductivity [cal/s/cm/°C]	6.24×10^{-4} @ 1.406 g cm ⁻³ ^[13]																				
Hardness	2.1 (Moh's scale) ^[13]																				
Hess brisance	16 mm ^[55]																				
Combustion T [K]	Burn rate and equilibrium combustion temperature ^[57] : $T_e = 2,475$ K, $m = 0.945$ g cm ⁻² s ⁻¹ (100 atm.) ^[57]																				
Specific volume	0.423 cc/g (@ 1.76 g cm ⁻³ , calcd., Mader) ^[19] , 0.714 cc/g (@ 1.00 g cm ⁻³ , calcd., Mader) ^[19]																				
Manometric bomb	2,350 kg/cm ² (@ 0.2 g cm ⁻³ , pressure formed on explosion in manometric bomb) ^[36] , 2,210–2,310 kg/cm ² (@ 0.20 g cm ⁻³ , manometric bomb) ^[36, 38] , 3,230 kg/cm ² (@ 0.25 g cm ⁻³ , manometric bomb) ^[36, 38]																				

	PA ^[3]	PA ^[21]	PA ^[22, 23]	PA ^[24]	PA ^[25]
Chemical formula	C ₆ H ₃ N ₃ O ₇	C ₆ H ₃ N ₃ O ₇	C ₆ H ₃ N ₃ O ₇	C ₆ H ₃ N ₃ O ₇	C ₆ H ₃ N ₃ O ₇
Molecular weight [g mol ⁻¹]	229.10	229.10	229.10	229.10	229.10
Crystal system	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic
Space group	<i>Pca</i> 2 ₁ (no. 29)	<i>Pca</i> 2 ₁ (no. 29)	<i>Pca</i> 2 ₁ (no. 29)	<i>Pca</i> 2 ₁ (no. 29)	<i>Pca</i> 2 ₁ (no. 29)
<i>a</i> [Å]	9.2548	9.254(2)	9.262(1)	9.1849(9)	9.1295(2)
<i>b</i> [Å]	19.1408	19.127(4)	19.137(1)	18.8333(19)	18.6869(5)
<i>c</i> [Å]	9.7134	9.704(2)	9.714(1)	9.8061(99)	9.7902(2)
α [°]	90	90	90	90	90
β [°]	90	90	90	90	90
γ [°]	90	90	90	90	90
<i>V</i> [Å ³]	1,720.6740	1,717.62	1,721.78	1,696.3(3)	1,670.23(7)
<i>Z</i>	8	8	8	8	8
ρ_{calc} [g cm ⁻³]					
<i>T</i> [K]					

Orthorhombic crystals obtained from EtOH.

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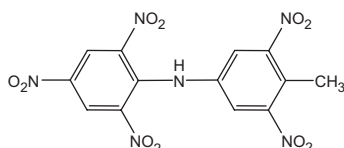
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4-Picrylamino-2,6-dinitrotoluene

Name [German, acronym]: Picrylamino dinitrotoluene, [4-picrylamino-2,6-dinitrotoluol, PADNT]

Main (potential) use: Useful for safe and insensitive explosive/propellant formulations^[1, 2, 4]

Structural formula:



	PADNT		
Formula	$C_{13}H_8N_6O_{10}$		
Molecular mass [g mol ⁻¹]	408.24		
Appearance at RT	Yellow crystalline solid ^[2]		
IS [J]	135 cm ^[1, 4] , $H_{50\%} = 135$ cm (2 kg mass) ^[2] , 97 cm (calcd., EDPHT 3.0) ^[3]		
FS [N]	Insensitive up to 36 kg (Julius-Peters apparatus) ^[2]		
N [%]	20.59		
$\Omega(\text{CO}_2)$ [%]	-78.39		
$T_{\text{m.p.}}$ [°C]	198–201 (open capillary, uncorrected) ^[1, 2] , 201 (endo, DTA @ 10 °C/min, static air, 10 mg sample) ^[2] , 198–201 ^[4]		
$T_{\text{dec.}}$ [°C]	299 (exo, DTA @ 10 °C/min, static air, 10 mg sample) ^[2]		
ρ [g cm ⁻³]	1.85 (density bottle method) ^[1, 2] , 1.718 (calcd. crystal ρ , calcd., EDPHT 2.0) ^[3] , 1.682 (calcd. crystal ρ , Ammon's method) ^[3] , 1.85 ^[4]		
Heat of formation			
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^\circ$ [kJ kg ⁻¹]			
T_{ex} [K]			
$p_{\text{C-1}}$ [kbar]		203.17 (@ 1.85 g cm ⁻³ , calcd.) ^[2]	

VoD [m s ⁻¹]		6,628 (@ 1.85 g cm ⁻³ , calcd.) ^[2]	
V ₀ [L kg ⁻¹]			
5 s explosion <i>T</i> [°C] Deflagration <i>T</i> [°C]	294 ^[2]		
Solubility [g/mL]	Recryst. from ethyl acetate ^[2]		

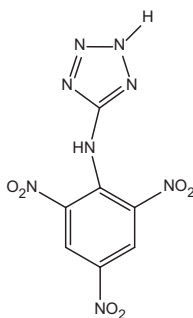
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5-Picrylamino-1,2,3,4-tetrazole

Name [German, acronym]: 5-(Picrylamino)tetrazole, picrylaminitetrazole
[picrylaminitetrazol, PAT]

Main (potential) use: Possible future lead-free initiator^[2]

Structural formula:



	PAT		
Formula	$C_7H_4N_8O_6$		
Molecular mass [g mol ⁻¹]	682.44		
Appearance at RT	Dark red solid ^[1]		
IS [J]	>50 cm (ball and disc test) ^[2] , $H_{50\%} = 36$ cm ^[2]		
FS [N]	>3.7 m/s (Emery paper test) ^[2]		
ESD [J]	1.0 ^[1] , ignition @ 0.45 but not @ 0.045 (standard test) ^[2]		
<i>N</i> [%]	29.01		
$\Omega(CO_2)$ [%]	-23.45		
$T_{m.p.}$ [°C]	77 (endo, DSC) ^[1]		
$T_{dec.}$ [°C]	210 (exo, peak max., DSC) ^[1]		
ρ [g cm ⁻³]	1.91 ^[2]		
Heat of formation	452.23 kJ/mol (calcd.) ^[1]		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{ex}U^\circ$ [kJ kg ⁻¹]			
T_{ex} [K]			
p_{C-J} [kbar]			

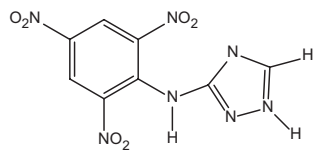
VoD [m s ⁻¹]			
V ₀ [L kg ⁻¹]			
5 s explosion <i>T</i> [°C] Ignition <i>T</i> [°C] Explosion <i>T</i> [°C]	214 ^[2] 210 (DTA) ^[2]		

	PAT^[1]
Chemical formula	C ₇ H ₈ N ₈ O ₆ •5H ₂ O
Molecular weight [g mol ⁻¹]	682.44
Crystal system	Monoclinic
Space group	<i>P</i> 2 ₁ / <i>c</i>
<i>a</i> [Å]	18.6978(11)
<i>b</i> [Å]	12.23850(13)
<i>c</i> [Å]	13.6407(12)
<i>α</i> [°]	90
<i>β</i> [°]	110.702(3)
<i>γ</i> [°]	90
<i>V</i> [Å ³]	2,919.9(3)
<i>Z</i>	1.552
<i>ρ</i> _{calc} [g cm ⁻³]	4
<i>T</i> [K]	291

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3-Picrylamino-1,2,4-triazole

Name [German, acronym]: 3-Picrylamino-1,2,4-triazole, [3-picrylamino-1,2,4-triazol, PATO]
Main (potential) use: Possible replacement for TATB, thermally stable explosive^[6]
Structural formula:



	PATO		
Formula	C ₈ H ₅ N ₇ O ₆		
Molecular mass [g mol ⁻¹]	295.17		
Appearance at RT			
IS [J]	>320 cm (2.5 kg mass) ^[2, 6, 9] , 145 (Rotter Fol) ^[3] , 320+ cm ^[10]		
FS [N]	>6 (Rotary friction FoF) ^[3]		
N [%]	32.22		
Ω(CO ₂) [%]	−67.76		
T _{m.p.} [°C]	310 ^[2, 6, 8, 10] , 315.6 ^[3] , 304.5 (dec., crude PATO) ^[9] , 310 (recryst. from γ-butyrolactone) ^[9] , 310 (dec.) ^[13]		
T _{dec.} [°C]	304.5 (crude PATO) ^[9] , 310 (one recryst. from γ-butyrolactone) ^[9] , 300 (DTA) ^[10]		
ρ [g cm ⁻³]	1.94 (crystal) ^[1, 2, 6] , 1.82 ^[3] , 1.936 (crystal) ^[9] , 1.82 (crystal) ^[10] , 1.936 ^[13]		
Heat of formation	36.3 kcal mol ⁻¹ (ΔH°) ^[1, 13] , 151.5 kJ/mol (enthalpy of form., exptl.) ^[12] , 149.6 kJ/mol (enthalpy of form., calcd., emp.) ^[12] , 112.5 kJ/mol (enthalpy of form., calcd., S-D method) ^[12]		
Heat of combustion	−959.5 kcal mol ⁻¹ ^[1] , ΔH° _c = −959.5 kcal/mol ^[13]		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
−Δ _{ex} U° [kJ kg ⁻¹]			
T _{ex} [K]			

p_{C-J} [kbar]		281 (calcd., K-J) ^[1] 307 (calcd.) ^[3] 307 (@ 1.936 g cm ⁻³ , calcd., BKW) ^[9] 24.7 GPa ^[10]	
VoD [m s ⁻¹]		7,780 (@ 1.94 g cm ⁻³ , calcd. K-J) ^[1] 7,850 (@ 1.936 g cm ⁻³ , calcd., BKW) ^[9]	
V_0 [L kg ⁻¹]			
Critical T [°C]	280–282 (exptl.) ^[4, 7] , 288 (calcd.) ^[4, 7] , 281 ± 1 (T_m) ^[13]		
Thermal stability	Thermally stable up to 300 °C (DTA and pyrolysis studies) ^[9]		
Vacuum stability test [cm ³ /h]	<p>@ 200 °C, total gas evolved (cm³/g) @ STP/time of exposure (days)^[5]: 1.0/2, 1.9/7, 2.8/14, 3.4/21, 4.0/28, 4.6/35, 5.2/42, 5.6/49, 6.1/56, 6.5/63, 7.2/70, 7.7/77, 8.7/84, 10.7/91^[5]</p> <p>@ 175 °C, total gas evolved (cm³/g) @ STP/time of exposure (days)^[11]: 0.1/2, 0.4/7, 0.6/14, 0.7/21, 0.8/28, 0.9/35, 1.1/42, 1.2/49, 1.3/56, 1.4/63, 1.4/70, 1.4/77, 1.4/84, 1.5/91^[11]</p>		

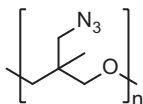
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Poly-3-azidomethyl-3-methyl-oxetane

Name [German, acronym]: Poly-3-azidomethyl-3-methyl-oxetane [poly-AMMO]

Main (potential) use: Energetic binder in composite propellants^[3]

Structural formula:



	Poly-AMMO (some data refer to structural unit)	
Formula	C ₅ H ₉ N ₃ O (AMMO)	
Molecular mass [g mol ⁻¹] Mean molecular weight [g mol ⁻¹]	127.15 1,000–3,000	
Appearance at RT		
IS [J]	>90 cm ^[2] , 1.0 Nm (1 kg hammer, 10 cm, very weak bang, AMMO) ^[5] , 7.5 Nm (5 kg hammer, 15 cm, ICT apparatus, very weak bang, poly-AMMO) ^[5] , 1.0 Nm (1 kg mass, 0.10 m drop height, very weak bang, ¹ / ₆ positive tests, AMMO monomer, liq., @ 20 °C, 51% air humidity) ^[7]	
FS [N]	160 (very weak crackling) ^[5] , 40 (tiny flames, ² / ₆ positive, AMMO monomer, liq., @ 20 °C, 51% air humidity) ^[7]	
N [%]	33.05	
Ω(CO ₂) [%]	–169.9	
T _{glass transition} [°C]	–46.5 ^[1] , –50 (oligo-AMMO, wt. = 1,030) ^[6] , –35 (poly-AMMO) ^[8]	
T _{dec.} [°C]	256 (DSC @ 5 °C/min) ^[1] , 220 (TGA @ 10 °C/min, first step) ^[1] , 232 (oligo-AMMO) ^[6]	
ρ [g cm ⁻³]	1.17 ^[3] , 1.24 (@ 293 K) ^[1] , 1.26 ^[2] , 1.17 (AMMO) ^[4] , 1.06 (poly-AMMO) ^[8]	
Heat of formation	43.9 kJ/mol (Δ _f H°), 345.19 kJ/kg (enthalpy of form.) ^[3] , 10.5 kcal/mol (ΔH _f , AMMO) ^[4] , 18 kJ/mol ^[8]	
	Calcd. (EXPLO5 6.03)	Exptl.
–Δ _{ex} U° [kJ kg ⁻¹]	2,506	
T _{ex} [K]	1,829	
p _{C-J} [kbar]	123	
VoD [m s ⁻¹]	6,069 (@ 1.7 g cm ⁻³)	
V ₀ [L kg ⁻¹]	763	

Thermal stability	81.6% mass loss @ 232 °C (dec. T, oligo-AMMO) ^[6]
Dec. enthalpy [J/g]	1,572 (oligo-AMMO) ^[6]

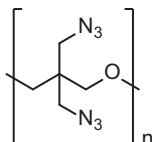
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Poly-3,3-bis-(azidomethyl)-oxetane

Name [German, acronym]: Poly-3,3-bis-(azidomethyl)-oxetane [poly-BAMO]*

Main (potential) use: Energetic binder in composite propellants

Structural formula:



*CE-BAMO is the abbreviation for chain-extended BAMO ($C_5H_{7.831}N_{5.396}O_{1.063}$)

	Poly-BAMO (some data refer to structural unit)
Formula	$C_5H_8N_6O$
Molecular mass [g mol ⁻¹] Mean molecular weight [g mol ⁻¹]	168.16 1,000–10,000
Appearance at RT	Colorless liquid (monomer) ^[5] , solid (poly-BAMO) ^[9]
IS [J]	>200 cm ^[2] , 5 Nm ^[4] , 1.0 Nm (1 kg hammer, 10 cm, ICT apparatus, very weak bang, BAMO) ^[7] , 10.0 Nm (5 kg hammer, 20 cm, very weak bang, poly-AMMO) ^[7] , 1.0 Nm (1 kg mass, 0.10 m drop height, very weak bang, BAMO monomer, liq., ² / ₆ positive, @ 20 °C, 51% air humidity) ^[10]
FS [N]	288 ^[4] , 60 (tiny flames, BAMO) ^[7] , 192 (very weak crackling, poly-BAMO) ^[7] , 60 (tiny flames, BAMO monomer, liq., ¹ / ₆ positive tests, @ 20 °C, 51% air humidity) ^[10]
N [%]	49.98 (monomer unit)
Ω(CO ₂) [%]	–123.69
T _{glass transition} [°C]	–39.2 ^[1] , –39 (poly-BAMO) ^[11] , –46 (oligo-BAMO, MWt. = 1,300) ^[8] , –45 (oligo-BAMO, MWt. = 1,420) ^[8] , –43 (oligo-BAMO, first heating, MWt. = 2,770) ^[8] , –42 (oligo-BAMO, second heating, MWt. = 2,770) ^[8] , –30 – –24 (poly-BAMO) ^[8]

$T_{\text{melt.}} [^{\circ}\text{C}]$	<p>60^[1]</p> <p>BAMO homopolymerization initiated by benzyl alcohol (BA) and $\text{BF}_3 \cdot \text{Et}_2\text{O}$ (as catalyst) in CH_2Cl_2^[7]:</p> <table border="1"> <thead> <tr> <th>mpt. ($^{\circ}\text{C}$)</th><th>Initiator</th><th>Ratio BAMO/BA</th><th>Repeated units</th><th>MW</th><th>Catalyst</th><th>Ratio of catalyst: initiator</th></tr> </thead> <tbody> <tr> <td>74.3</td><td>BA</td><td>3</td><td>13</td><td>2,184</td><td>$\text{BF}_3 \cdot \text{Et}_2\text{O}$</td><td>2</td></tr> <tr> <td>65.78</td><td>BA</td><td>6</td><td>25</td><td>4,200</td><td>$\text{BF}_3 \cdot \text{Et}_2\text{O}$</td><td>2</td></tr> <tr> <td>72.0</td><td>BA</td><td>6</td><td>29</td><td>4,872</td><td>$\text{BF}_3 \cdot \text{Et}_2\text{O}$</td><td>2</td></tr> <tr> <td>78.24</td><td>BA</td><td>30</td><td>58</td><td>9,744</td><td>$\text{BF}_3 \cdot \text{Et}_2\text{O}$</td><td>2</td></tr> </tbody> </table> <p>70–90 (poly-BAMO, range, depending on thermal treatment)^[8], 47 (oligo-BAMO, MWt. = 1,300), 53 (oligo-BAMO, MWt. = 1,420)^[8], 61–71 (oligo-BAMO, first heating, MWt. = 2,770)^[8], 48–61 (oligo-BAMO, second heating, MWt. = 2,770)^[8]</p>						mpt. ($^{\circ}\text{C}$)	Initiator	Ratio BAMO/BA	Repeated units	MW	Catalyst	Ratio of catalyst: initiator	74.3	BA	3	13	2,184	$\text{BF}_3 \cdot \text{Et}_2\text{O}$	2	65.78	BA	6	25	4,200	$\text{BF}_3 \cdot \text{Et}_2\text{O}$	2	72.0	BA	6	29	4,872	$\text{BF}_3 \cdot \text{Et}_2\text{O}$	2	78.24	BA	30	58	9,744	$\text{BF}_3 \cdot \text{Et}_2\text{O}$	2
mpt. ($^{\circ}\text{C}$)	Initiator	Ratio BAMO/BA	Repeated units	MW	Catalyst	Ratio of catalyst: initiator																																			
74.3	BA	3	13	2,184	$\text{BF}_3 \cdot \text{Et}_2\text{O}$	2																																			
65.78	BA	6	25	4,200	$\text{BF}_3 \cdot \text{Et}_2\text{O}$	2																																			
72.0	BA	6	29	4,872	$\text{BF}_3 \cdot \text{Et}_2\text{O}$	2																																			
78.24	BA	30	58	9,744	$\text{BF}_3 \cdot \text{Et}_2\text{O}$	2																																			
$T_{\text{dec.}} [^{\circ}\text{C}]$	186.9 (DTA) ^[1] , 261 (DSC) ^[3] , 219 (DTA @ 10 $^{\circ}\text{C}/\text{min}$, oligo-BAMO, MWt. = 2,770) ^[8] , ~250 (DSC @ 10 $^{\circ}\text{C}/\text{min}$, oligo-BAMO, MWt. = 2,770) ^[8]																																								
$T_{\text{b.p.}} [^{\circ}\text{C}]$	67 @ 0.25 mm (monomer) ^[5] , 79–81 @ 0.4 mm (monomer) ^[5]																																								
$\rho [\text{g cm}^{-3}]$	1.30 (poly-BAMO) ^[11] , 1.270 (BAMO copolymer) ^[12] , 1.25 ^[4] , $d^{25} = 1.22$ (monomer) ^[5] , 1.3 (@ 293 K) ^[1] , 1.30 (BAMO) ^[6] , 1.29 (CE-BAMO) ^[6]																																								
Heat of formation	2,460 kJ/kg ^[1] , 2,460.8 kJ/kg (enthalpy of form.) ^[4] , 102 kcal/mol (calcd., monomer) ^[5] , 100.3 kcal/mol (ΔH_f , BAMO) ^[6] , 103.5 (ΔH_f , CE-BAMO) ^[6] , 2,209 kJ/kg (poly-BAMO) ^[9] , 413 kJ/mol (poly-BAMO) ^[11] , 2.46 MJ/kg (@ 293 K, BAMO prepolymer) ^[12] , 1.19 MJ/kg (@ 293 K, BAMO copolymer) ^[12]																																								
	Calcd. (EXPLO5 6.03)			Exptl.																																					
$-\Delta_{\text{ex}}U^{\circ} [\text{kJ kg}^{-1}]$	3,982																																								
$T_{\text{ex}} [\text{K}]$	2,544																																								
$p_{\text{C-J}} [\text{kbar}]$	134																																								
$\text{VoD} [\text{m s}^{-1}]$	6,753																																								
$V_0 [\text{L kg}^{-1}]$	78																																								

Thermal stability	91.7% (loss of mass @ dec. T) ^[8]
Burn rate [mm/s]	Approx. values from graph for BAMO co-polymer: 1.4 mm/s @ 7.2 mol/mg N_3 bond density ^[12] , 1.9 mm/s @ 8.0 mol/mg N_3 bond density ^[12] , 3.0 mm/s @ 8.4 mol/mg N_3 bond density ^[12] , 4.0 mm/s @ 8.9 mol/mg N_3 bond density ^[12]

Melting enthalpy [J/g]	−7.3 (oligo-BAMO, MWt. = 1,300) ^[8] , −24.8 (oligo-BAMO, MWt. = 1,420) ^[8] , −34.8 (oligo-BAMO, MWt. = 2,770, first heating) ^[8] , −12.6 (oligo-BAMO, MWt. = 2,770, second heating) ^[8]
Decomposition enthalpy [J/g]	2,625 (oligo-BAMO) ^[8]
ΔC_p [J/g K]	0.57 (oligo-BAMO, MWt. = 1,300) ^[8] , 0.32 (oligo-BAMO, MWt. = 1,420) ^[8] , 0.28 (oligo-BAMO, MWt. = 2,770, first heating) ^[8] , 0.50 (oligo-BAMO, MWt. = 2,770, second heating) ^[8]
Flame T [K]	2,020 (@ 10 MPa, BAMO pre-polymer) ^[12] , 1,520 (@ 10 MPa, BAM copolymer) ^[12]

	oligo-BAMO^[8]
Chemical formula	
Molecular weight [g mol ^{−1}]	2,770
Crystal system	Monoclinic
Space group	
a [Å]	10.907(7)
b [Å]	7.5046(16)
c [Å]	6.150(3)
α [°]	90
β [°]	100.58(4)
γ [°]	90
V [Å ³]	494.8(5)
Z	
ρ_{calc} [g cm ^{−3}]	
T [K]	

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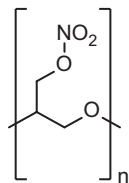
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Poly-GLYN

Name [German, acronym]: Poly-GLYN, poly(glycidyl nitrate) [poly-GLYN, poly glyn, PGN]

Main (potential) use: Energetic binder in composite propellants

Structural formula:



* currently poly-GLYN is produced in two molecular weight ranges: (i) standard with MW 1,000–2,000 and M_n 750–1,100 and (ii) longer chain with MW 2,000–3,500 and M_n 1,100–2,000. End-modified PolyGLYN is end-modified using the sulfuric acid hydrolysis process

	Poly-GLYN (some data refer to structural unit)	
Formula	C ₃ H ₅ NO ₄	
Molecular mass [g mol ⁻¹]	119.08	
Mean molecular weight [g mol ⁻¹]	(ideal mol. wt. = 1,500 g/mol) ^[5]	
Appearance at RT		
IS [J]	>200 cm ^[2]	
N [%]	11.76	
Ω(CO ₂) [%]	-60.46	
T _{glass transition} [°C]	-35 ^[1, 5]	
T _{dec.} [°C]		
ρ [g cm ⁻³]	1.39 (PGN) ^[1] , 1.47 ^[4] , 1.45 ^[5]	
Heat of formation	-68 kcal/mol ^[5] , 2.71 kJ/g (Δ _f H°, prepolymer) ^[3] , -2.244 kJ/g (Δ _f H°, calcd., CHEETAH 2.0, pre-polymer) ^[3] , -2.389 kJ/g (Δ _f H°) ^[3] , -2,586 kJ/kg (poly-GLYN) ^[4] , -285 kJ/mol (poly-GLYN) ^[1]	
Heat of combustion	14.7 kJ/g (ΔH _c) ^[3]	
	Calcd. (EXPLO5 6.03)	Exptl.
-Δ _{ex} U° [kJ kg ⁻¹]	6,100	
T _{ex} [K]	3,863	
p _{C-J} [kbar]	207	
VoD [m s ⁻¹]	7,253	
V ₀ [L kg ⁻¹]	819	

5 s explosion T [°C] Ignition T [°C]	170 ^[5]
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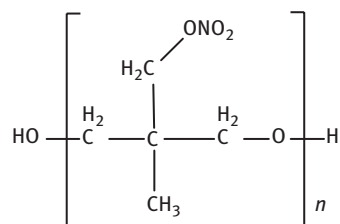
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Poly(3-nitratomethyl-3-methyloxetane)

Name [German, acronym]: Poly(3-nitratomethyl-3-methyloxetane) [polyNIMMO]

Main (potential) use: Energetic polymer^[9], energetic binder^[8], promising energetic binder for insensitive munitions^[8], can be used as energetic binder in low vulnerability gun propellants, high-impulse rocket propellants, elastomer-modified double-base propellants and high energy PBXs^[9]

Structural formula:



	polyNIMMO
Formula	C ₅ H ₉ NO ₄ (monomer)
Molecular mass [g mol ⁻¹]	147.12 (monomer)
Appearance at RT	Highly viscous, yellow transparent liquid with slight odor (uncured material) ^[8]
IS [J]	
FS [N]	
ESD [J]	
N [%]	9.52 (monomer)
Ω(CO ₂) [%]	-114.18 (monomer)
T _{glass transition} [°C]	-15.1 (DSC @ 10 °C/min, midpoint) ^[4] , -33.0 (DSC) ^[7] , -15 (DSC) ^[1] , -15 ^[2] , 258.2 K ^[2] , -25 (polyNIMMO) ^[6] , ~-33 (polyNIMMO) ^[8]
T _{dec.} [°C]	216.47 (exo, peak max. (dec. in range 195–225 °C), DSC @ 10 K/min) ^[8]
ρ [g cm ⁻³]	1.26 ^[5–7]
Heat of formation	335 kJ/mol (poly-NIMMO) ^[6] , -2.29 kJ/g (prepolymer) ^[3] , -0.39 kJ/g (prepolymer, Colclough) ^[3] , -2.101 kJ/g (prepolymer, <i>Cumming</i>) ^[3] , -2,101.5 kJ/kg (heat of formation, poly-NIMMO) ^[5]

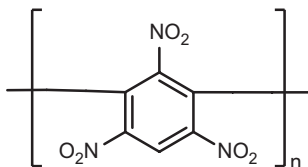
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.																				
$-\Delta_{\text{ex}}U^{\circ}$ [kJ kg ⁻¹]																							
T_{ex} [K]																							
$p_{\text{C-J}}$ [kbar]																							
VoD [m s ⁻¹]																							
V_0 [L kg ⁻¹]																							
5 s explosion T [°C] Deflagration T [°C]	193 (DSC @ 20 °C/min) ^[4]																						
Thermal stability	Decomposes to form gases on aging leading to voids in explosive composition ^[9] , prepolymer polyNIMMO ages naturally with time even @ ambient T and dec. is accelerated by increasing T ^[9] , pyrolysis >90 °C results in darker color and increase in viscosity with longer heating times ^[9]																						
Viscosity [cP]	234.80 Pa s ^[4] <table border="1"> <thead> <tr> <th>Viscosity^[1] (cP)</th><th>T (°C)</th><th>Viscosity^[1] (cP)</th><th>T (°C)</th></tr> </thead> <tbody> <tr> <td>~320,000</td><td>25</td><td>~ 50,000</td><td>45</td></tr> <tr> <td>~190,000</td><td>30</td><td>~ 20,000</td><td>50</td></tr> <tr> <td>~120,000</td><td>35</td><td>~ 10,000</td><td>55</td></tr> <tr> <td>~70,000</td><td>40</td><td>~ 5,000</td><td>60</td></tr> </tbody> </table> <p>Viscosity of plasticizer/binder blend increases: BDNPA < BTTN < DNDA-57 < BuNENA \approx DEGDN^[87]</p>			Viscosity ^[1] (cP)	T (°C)	Viscosity ^[1] (cP)	T (°C)	~320,000	25	~ 50,000	45	~190,000	30	~ 20,000	50	~120,000	35	~ 10,000	55	~70,000	40	~ 5,000	60
Viscosity ^[1] (cP)	T (°C)	Viscosity ^[1] (cP)	T (°C)																				
~320,000	25	~ 50,000	45																				
~190,000	30	~ 20,000	50																				
~120,000	35	~ 10,000	55																				
~70,000	40	~ 5,000	60																				
Dutch test	0.45% (105 °C, 72 h) ^[4]																						
Decomposition energy [J/g]	1,300 (DSC) ^[7]																						
Radiation sensitivity	Very stable to gamma radiation up to doses of 250 kGy ^[8, 9] , radicals produced @ 250 kGy but are short lived and do not result in structural changes, whereas @ 750 kGy structural changes occur ^[9] , easily decomposes if subjected to UV radiation ^[9]																						
Compatibility	Compatible (A rating) with BTTN, DNDA-57, DEGDN, BuNENA, BDNPA based on shift of T_{dec} in DSC (T_{dec} (exo peak max., DSC @ 10 K/min, poly-NIMMO with 20% energetic plasticizer): 216.47 (poly-NIMMO), 215.53 (poly-NIMMO + BDNPA), 216.33 (poly-NIMMO + BuNENA), 217.13 (poly-NIMMO + DEGDN), 214.60 (poly-NIMMO + BTTN), 215.50 (poly-NIMMO + DNDA-57) ^[8]																						
Photosensitivity	Easily decomposes if subjected to UV radiation ^[9]																						

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Polynitropolyphenylene

Name [German, acronym]: Polynitrophenylene [polynitropolyphenylen, PNP]
 Main (potential) use: Energetic binder, heat resistant but extremely impact sensitive energetic binder^[3], caseless munition^[3], high ignition temperature propellants^[3], possible future high-temperature resistant explosive binding agent^[4]

Structural formula:



	PNP (some data refer to structural unit)																															
Formula	C ₆ HN ₃ O ₆																															
Molecular mass [g mol ⁻¹] Mean molecular weight [g mol ⁻¹]	211.09 2,350, (GPC mol. wt. = ~2,000 g/mol) ^[3]																															
Appearance at RT	Amorphous green, yellow-brown powder ^[3] , green, brownish-yellow solid mass, noncrystalline (polymer) ^[4]																															
IS [J]	4 ^[1, 4] , 4 (BAM) ^[3]																															
FS [N]	360 ^[1] , 240 (no go, BAM) ^[3] , 360 (weak, sizzling) ^[4] , 240 (no reaction) ^[4]																															
N [%]	19.91																															
Ω(CO ₂) [%]	−49.30																															
T _{m,p.} [°C]	Does not melt (polymer) ^[4] , no endotherm in DSC (polymer) ^[4]																															
T _{dec.} [°C]	280–304 (DSC @ 5 °C/min), 250 (DTA @ 5 °C/min) ^[1, 3] DTA/TGA, Mettler TA 200 C apparatus ^[4] : <table><tr><th rowspan="2">Heating rate (K/min)</th><th colspan="2">Exothermal dec. (°C)</th><th colspan="5">Weight reduction @ °C</th></tr><tr><th>Start</th><th>Peak max</th><th>Start</th><th>1%</th><th>5%</th><th>10%</th><th>20%</th></tr><tr><td>10, N₂</td><td>248</td><td>298</td><td>200</td><td>253</td><td>276</td><td>287</td><td>292 (deflag.)</td></tr><tr><td>5, N₂</td><td>250</td><td>317</td><td>190</td><td>256</td><td>284</td><td>292</td><td>301</td></tr></table>	Heating rate (K/min)	Exothermal dec. (°C)		Weight reduction @ °C					Start	Peak max	Start	1%	5%	10%	20%	10, N ₂	248	298	200	253	276	287	292 (deflag.)	5, N ₂	250	317	190	256	284	292	301
Heating rate (K/min)	Exothermal dec. (°C)		Weight reduction @ °C																													
	Start	Peak max	Start	1%	5%	10%	20%																									
10, N ₂	248	298	200	253	276	287	292 (deflag.)																									
5, N ₂	250	317	190	256	284	292	301																									

ρ [g cm ⁻³]	1.8–2.2 (@ 293 K) ^[1] , 1.8–2.2 ^[4] , 520 (bulk ρ) ^[4]	
Heat of formation	–65.2 kJ/mol ($\Delta_f H^\circ$) ^[1] , –309 kJ/kg ($\Delta_f H^\circ$) ^[1]	
	Calcd. (EXPLO5 6.03)	Exptl.
$-\Delta_{\text{ex}} U^\circ$ [kJ kg ⁻¹]	4,549	3,200 [H ₂ O (l)] ^[2] 3,300 (explosion energy, 25 mL bomb, loading $\rho = 100$ kg/m ³) ^[4]
T_{ex} [K]	3,616	
$p_{\text{C-J}}$ [kbar]	236	
VoD [m s ⁻¹]	7,538	
V_0 [L kg ⁻¹]	606	

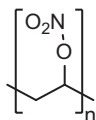
5 s explosion T [°C] Deflagration T [°C]	286–294 (50 mg sample, @ 20 K/min, polymer) ^[4] , 304 (50 mg sample, @ 20 K/min, improved purity sample, polymer) ^[4] , 292 \pm 300 (TGA, polymer) ^[4]
Thermal stability	1.349 mL gas evolved after 40 h @ 125 °C (polymer) ^[4]
Solubility [g/mL]	Readily soluble in organic solvents such as acetone and ethyl acetate ^[3, 4]
Compatibility	Compatible with HMX ^[4]
Steel case test	20 mm nozzle diameter, fragment pattern F, explosion time = 9 s (confined in steel case Rn 1154 GGVE) ^[4] , 24 mm nozzle diameter, fragment pattern B, deflagration time = 10 s (confined in steel case Rn 1154 GGVE) ^[4]
Flame sensitivity	Burns immediately (soot generation, ignition by match) ^[4] , burns immediately (soot generation, 10 mm high, 5 mm wide gas flame) ^[4] , 0.5 g PNP ignited immediately and burned with 20 cm high sooty flame, duration of 1–2 s (red-hot steel dish) ^[4]

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Polyvinyl nitrate

Name [German, acronym]: Polyvinyl nitrate, polyvinyl alcohol nitrate [polyvinylnitrat, PVN]
 Main (potential) use: Plasticizer for TNT^[4], few applications due to poor chemical stability^[8], PVN dissolved in mononitrotoluene is used as an additive to TNT charges since it improves the crystallinity structure of the TNT cast^[10]

Structural formula:



	PVN (data refer to structural unit)
Formula	$(\text{C}_2\text{H}_3\text{NO}_3)_n$
Molecular mass [g mol ⁻¹] Mean molecular weight [g mol ⁻¹]	89.05 (@ degree of substitution 1) ^[10] 200,000
Appearance at RT	Pale yellow brown ^[10]
IS [J]	10 Nm ^[4] , 1.99 (4 in, 2 kg mass, P.A. for 14.86% N) ^[11] , 30–35 cm (cf. 158 cm for TNT, Rotter apparatus) ^[5] , 4 in (2 kg mass, P.A. for 14.86% N) ^[5]
FS [N]	196 ^[4] , crackles with steel shoe (friction pendulum test) ^[11] , unaffected by fiber shoe (friction pendulum test) ^[11]
N [%]	15.73 (@ degree of substitution 1) ^[10] , usually 13.5–14.5% with theoretical max. of 15.75% ^[11]
Ω(CO ₂) [%]	–44.9 (@ degree of substitution 1) ^[10]
T _{m,p.} [°C]	50 ^[11] , (softening point = 30–50 °C) ^[5] , nonmeltable ^[11]
T _{dec.} [°C]	175, (deflagration point = 175) ^[5]
ρ [g cm ⁻³]	1.6 ^[4]
Heat of formation	–102.6 kJ/mol (Δ _f H°), –1,152.1 kJ/kg (enthalpy of form.) ^[4] , –1,152 kJ/kg (ΔH _f , ICT thermochemical database) ^[9] , –275.6 kcal/kg (Q _f ^V) ^[5] , –102.59 kJ/mol (enthalpy of form., PVN with 15.73% N content) ^[10] , –102.6 kJ/mol (enthalpy of form., exptl.) ^[12] , –154.3 kJ/mol (enthalpy of form., calcd., emp.) ^[12] , –150.2 kJ/mol (enthalpy of form., calcd., S-D method) ^[12]

	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^\circ$ [kJ kg ⁻¹]	5,357	4,781 J/g (calcd., ICT-code) ^[9] 4,782 J/g [H ₂ O (l)] (calcd. thermodynamically, 15.73% N content) ^[10] 4,490 J/g [H ₂ O (g)] (calcd. thermodynamically, 15.73% N content) ^[10]	3,766 ^[1] 4,574 ^[3] 4,781 [H ₂ O (l)] ^[4] 4,490 [H ₂ O (g)] ^[4] 1,180 kcal/kg ^[5] 900 kcal/kg ^[1, 6] 900 kcal/kg (for PVN with 14.86% N content) ^[5]
T_{ex} [K]	3,559	3,388 (calcd., ICT-code) ^[9]	
$p_{\text{C-J}}$ [kbar]	235	143.0 MPa (calcd., ICT-code) ^[9]	
VoD [m s ⁻¹]	7,563 (@ 1.5 g cm ⁻³) ^[4]		2,030 (@ 0.3 g cm ⁻³ , PVN containing 13.4% N, cardboard cartridge, 30 mm diameter) ^[5, 8, 11] 3,450–3,520 (@ 0.6 g cm ⁻³ , PVN containing 13.4% N, cardboard cartridge, 30 mm diameter) ^[5, 8, 11] 4,920–5,020 (@ 1.0 g cm ⁻³ , PVN containing 13.4% N, cardboard cartridge, 30 mm diameter) ^[5, 8, 11] 6,090 (@ 1.4 g cm ⁻³ , PVN containing 13.4% N, cardboard cartridge, 30 mm diameter) ^[5, 8, 11] 6,560 (@ 1.5 g cm ⁻³ , PVN containing 13.4% N, cardboard cartridge, 30 mm diameter) ^[5, 8, 11]
V_0 [L kg ⁻¹]	755		838 ^[1] 958 ^[2, 4] 1,009 ^[3] 833 (for PVN with 14.86% N content) ^[5]

Trauzl test [cm ³ , % TNT]	153–341 cc (cf. 255 cc for TNT) ^[5] , 113.5 cc (low viscosity PVN, max. N content = 14.48%) ^[5] , 102 cc (high viscosity PVN, max. N content = 13.43%) ^[5] , 153–342 cm ³ (PVN, 13–15% N content) ^[8, 11]
Sand test [g]	49.9 g (200 g bomb) ^[1] , 104–107% TNT ^[7] , 49.9 g sand crushed (200 g bomb, cf. 48.0 g for TNT; for PVN with 14.86% N content) ^[5]
5 s explosion <i>T</i> [°C] 5 s ignition <i>T</i> [°C] Ignition <i>T</i> [°C] Autoignition <i>T</i> [°C]	265 (for PVN with 14.86% N content) ^[1, 5] 265 ^[6] 160–178 ^[5] 188–190 (0.2 g sample, @ 5 °C/min, Wood's metal bath, PVN with 14.9% N, degree of substitution of 0.90) ^[10]
100 °C heat test [% mass loss]	1.9% mass loss in first 48 h ^[1, 5] , 2.1% in second 48 h ^[1, 5] , no explosions in 100 h (for PVN with 14.86% N content) ^[1, 5]
Thermal stability	<0.3% mass loss (2 days @ 75 °C, closed vials for PVN with 14.86% N content) ^[10] , ~0.6% mass loss (5 days @ 75 °C, closed vials for PVN with 14.86% N content) ^[10] , ~0.8% mass loss (6 days @ 75 °C, closed vials for PVN with 14.86% N content) ^[10] , ~1.0% mass loss (8 days @ 75 °C, closed vials for PVN with 14.86% N content) ^[10] , <0.5% mass loss (2 days @ 75 °C, closed vials for PVN with 14.86% N content) ^[10] , 3% mass loss requires 17 years @ 30 °C (apparent time, predicted, PVN with 14.86% N content) ^[10] , 3% mass loss requires 10 years @ 30 °C (real time, predicted, PVN with 14.86% N content) ^[10]
Vacuum stability test [cm ³ /h]	>11 cc in 16 h @ 100 °C (for PVN with 14.86% N content) ^[1, 5] , >11 cc in 16 h @ 120 °C (for PVN with 14.86% N content) ^[1, 5] , 2.7 mL/g (40 h @ 90 °C, PVN with 14.86% N content) ^[10]
Burn rate [mm/s]	Readily inflammable, burns without melting ^[8] , flammable ^[11]
Adiabatic self-heating [°C]	Transition to deflagration @ 164 °C (ARCTM, PVN with 14.86% N content) ^[10]
Dec. activation energy [kJ/mol]	146 (PVN with 14.86% N content) ^[10]
Hygroscopicity	0.62% @ 30 °C with 90% RH ^[1]
65.5 °C KI test	60+ min ^[1]
34.5 °C heat test	Salmon pink, 20 minutes ^[1] , red fumes, 25 min ^[1] , explodes, 300+ min ^[1]
40 h hydrolysis test	5.07% HNO ₃ ^[1]

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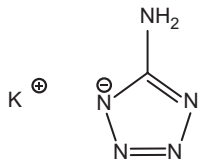
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Potassium 5-aminotetrazolate

Name [German, acronym]: Potassium aminotetrazolate, [kalium 5-aminotetrazolat]

Main (potential) use: In the synthesis of other energetic tetrazole compounds^[1]

Structural formula:



	Potassium 5-aminotetrazolate		
Formula	CH ₂ KN ₅		
Molecular mass [g mol ⁻¹]	123.16		
Appearance at RT	Colorless crystals ^[1, 3]		
IS [J]			
FS [N]			
ESD [J]			
N [%]	56.86		
Ω(CO ₂) [%]			
T _{m,p.} [°C]	263 (DSC @ 5 °C/min, covered Al pans) ^[1] , 267 ^[3]		
T _{dec.} [°C]			
ρ [g cm ⁻³]	1.961 (X-ray) ^[1]		
Heat of formation	−202 kJ/mol (ΔH _f ^o) ^[1]		
Heat of combustion	Δ _c H ^o = −763 kJ/mol ^[1] , Δ _c U = −1,484 cal/g (@ C ^v , exptl. bomb calorimetry) ^[1]		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
−Δ _{ex} U ^o [kJ kg ⁻¹]			
T _{ex} [K]			
p _{C-J} [kbar]			
VoD [m s ⁻¹]			
V _o [L kg ⁻¹]			
Solubility [g/mL]	Recryst. from hot H ₂ O/EtOH (1:4) ^[1]		
Flame test	Purple flame color ^[1]		

	Potassium aminotetrazolate ^[1, 2]
Chemical formula	KCH ₂ N ₅
Molecular weight [g mol ⁻¹]	123.18
Crystal system	Monoclinic
Space group	<i>P</i> 2 ₁ / <i>c</i> (no. 14)
<i>a</i> [Å]	6.8702(8)
<i>b</i> [Å]	9.8516(9)
<i>c</i> [Å]	6.8372(7)
α [°]	90
β [°]	115.6(1)
γ [°]	90
<i>V</i> [Å ³]	417.29(8)
<i>Z</i>	4
ρ_{calc} [g cm ⁻³]	1.961
<i>T</i> [K]	120
	Recryst. from hot H ₂ O/EtOH (1:4)

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Potassium chlorate

Name [German, acronym]: Potassium chlorate, potcrate [Kaliumchlorat]
Main (potential) use: Oxidizer for primer formulations and pyrotechnical compositions, common pyrotechnic oxidizer^[10]
Structural formula:



	Potassium chlorate	
Formula	KClO ₃	
Molecular mass [g mol ⁻¹]	122.6	
Appearance at RT	White powder ^[7] , white crystalline substance ^[8] , colorless crystals/white powder ^[10] , colorless, lustrous crystals or white granules/powder ^[11]	
IS [J]	2/6 positive @ 16 cm (2 kg mass) ^[5]	
N [%]	±0	
Ω(CO ₂) [%]	+39.2	
T _{phase transitions} [°C]	>523 K (monoclinic (phase I) → orthorhombic (phase-III)) ^[2] , phase I (monoclinic, distorted NaCl-type structure) is stable @ ambient conditions and transforms @ 257 °C to phase III (orthorhombic with distorted NaCl-type structure) ^[4] , when compressed, phase I transforms to phase II (~6% higher density phase) ^[4]	
T _{m,p.} [°C]	368–370 ^[5] , 368 ^[8, 11] , 370 ^[10]	
T _{dec.} [°C]	400 ^[5, 8] , above 368 °C dec. ^[11]	
ρ [g cm ⁻³]	2.32 ^[5, 8, 11] , 2.34 ^[10]	
Heat of formation	–93.5 kcal/mol (Q _f) ^[5] , –398 kJ/mol (enthalpy of form.) ^[10]	
	Calcd. (EXPLO5 6.04)	Exptl.
–Δ _{ex} U° [kJ kg ⁻¹]		
T _{ex} [K]		
p _{C-J} [kbar]		
VoD [m s ⁻¹]		
V ₀ [L kg ⁻¹]		

Trauzl test [cm ³ , % TNT]	No measureable value ^[5]
5 s explosion T [°C] Explosion T [°C]	Rapid heating may cause explosion ^[7]

Solubility [g/mL]	3.3 parts KClO ₃ per 100 parts H ₂ O @ 0 °C ^[6] , 56 parts KClO ₃ per 100 parts H ₂ O @ 100 °C ^[6] , moderately soluble in water ^[7] , slightly soluble in EtOH ^[7] , 8.6 g/100 g H ₂ O @ 25 °C ^[10] , 1 g dissolves slowly in 16.5 mL water ^[11] , 1 g dissolves in 1.8 mL boiling water ^[11] , 1 g dissolves in ~50 mL glycerol ^[11] , almost insoluble in EtOH ^[11]
Hygroscopicity	Not hygroscopic ^[6] , critical humidity = 98.0% RH @ 25 °C ^[9]
Compatibility	Can form explosive mixtures with combustible materials such as sulfur, charcoal, sugar and metal powders ^[10] , dec. catalyzed by MnO ₂ , [Co ₃ O ₄] or metal oxides of metals which have multiple oxidation states ^[10] , ammonium salts can result in formation of spontaneously explosive ammonium chlorate ^[10] , unstable in presence of acid ^[10] , incompatible with sulfides of antimony or arsenic (forms compositions highly IS and FS) ^[10] , incompatible with any soluble copper salts ^[10] , should be kept out of contact with organic substances or other oxidizable substances ^[11] , explodes with sulfuric acid ^[11] , inflames with explosion if triturated with organic substances, sulfur, phosphorus, sulfites, hypophosphite and other oxidizable substances ^[11] , incompatible with iodides and tartaric acid ^[11]
Enthalpy of dec. [kJ/mol]	−39 (assuming KClO ₃ → KCl + 1½ O ₂) ^[10]

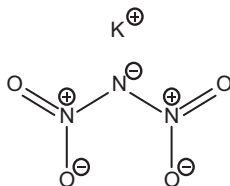
	Potassium chlorate ^[2]	Potassium chlorate ^[1]	Potassium chlorate ^[3]	Potassium chlorate ^[4]
	Phase-I	Phase-III	Phase-I	High-pressure phase-II
Chemical formula	KClO ₃	KClO ₃	KClO ₃	KClO ₃
Molecular weight [g mol ^{−1}]	122.6	122.6	122.6	122.6
Crystal system	Monoclinic	Orthorhombic	Monoclinic	
Space group	<i>P</i> 2 ₁ / <i>m</i> (no. 11)	<i>P</i> <i>c</i> <i>m</i> <i>n</i>	<i>P</i> 2 ₁ / <i>m</i> (no. 11)	<i>R</i> 3 <i>m</i> (no. 160)
<i>a</i> [Å]	4.630(2)	4.74	4.6569	4.273(10)
<i>b</i> [Å]	5.568(3)	5.64	5.59089	4.273(10)
<i>c</i> [Å]	7.047(3)	13.8	7.0991	4.273(10)
<i>α</i> [°]	90	90	90	85.5(2)
<i>β</i> [°]	110.21(3)	90	109.648	85.5(2)
<i>γ</i> [°]	90	90	90	85.5(2)
<i>V</i> [Å ³]		368.92		77.24
<i>Z</i>	2	4		
<i>ρ</i> _{calc} [g cm ^{−3}]				
<i>T</i> [K]	77	280 °C		25 °C, 112.5 kbar pressure

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Potassium dinitramide

Name [German, acronym]: Potassium dinitramide [kalium-dinitramid, KDN]
 Main (potential) use: Synthetic reagent for introducing the dinitramide ion into energetic compounds^[1], inorganic oxidant with potential applications in propellants and pyrotechnics^[9]

Structural formula:



	KDN
Formula	KN ₃ O ₄
Molecular mass [g mol ⁻¹]	145.12
Appearance at RT	White crystalline solid ^[9] , crystalline solid mainly small cubes with typical edge length of 200–300 μm ^[12]
IS [J]	>50 cm ^[1] , Fol =>145 ^[6] , >20 (mean particle diameter of sample = 256 μm) ^[11]
FS [N]	0 ^[2] , >360 (BAM) ^[6] , >360 (mean particle diameter of sample = 256 μm) ^[11]
ESD [J]	142.53 mJ ^[2] , 4.5 ^[6] , >5.6 (mean particle diameter of sample = 256 μm) ^[11]
N [%]	28.96
Ω(CO ₂) [%]	
T _{m,p.} [°C]	124–126 ^[1] , 128 ^[2] , 127–131 ^[15, 12] , movt. in sample >90 °C, fusion of salt ~ 130 °C (thermomicroscopy) ^[9] , 130 (DSC @ 20 °C/min, sealed tubes) ^[9] , 130 ^[10] , 130 (strong endo peak, DSC, mean particle diameter of sample = 256 μm) ^[11] , 125–129 (small scale) ^[12] , 126–131 (large scale) ^[12] , 127 ^[12] , 125 (DSC/TGA @ 5 K/min) ^[12]

$T_{\text{dec.}} [^{\circ}\text{C}]$	<p>238^[3], 105 (small exotherm), 108 (small endotherm), 128 (large endotherm) (DSC @ 5 $^{\circ}\text{C}/\text{min}$)^[5, 6]; 92–108 (exotherm, breakdown of crystal structure), 109–115 (partial melting), 119 (melting, onset) (hot-stage microscopy)^[5, 6], 108 (endotherm, mpt. of KDN/KNO_3 eutectic), 140–182 (two overlapping exotherm maxima)^[5], 227 (exotherm), 319 (endotherm, KNO_3 melting) (DSC)^[5, 6], movt. in sample >90 $^{\circ}\text{C}$, fusion of salt ~ 130 $^{\circ}\text{C}$, bubbles in melt >150 $^{\circ}\text{C}$ (thermomicroscopy)^[9], >200 (DSC @ 20 $^{\circ}\text{C}/\text{min}$, sealed tubes)^[9], 160 (onset, two-stage dec., ~38% mass loss in first stage dec.)^[10], 220–230 (strong exo peak, DSC, mean particle diameter of sample = 256 μm)^[11], two-step weight loss @ 90 $^{\circ}\text{C}$ and 180 $^{\circ}\text{C}$ (total weight loss = 39%, DSC/TGA @ 5 K/min)^[12]</p> <p>DSC, Al crucible with pinhole in lid, Ar atmosphere, 10 $^{\circ}\text{C}/\text{min}$, 2.5 mg sample, T_e = extrapolated value, T_p = peak value^[9]:</p> <table> <tr> <th rowspan="2">KDN type</th><th colspan="2">Fusion (melting)</th><th colspan="4">Decomposition</th></tr> <tr> <th>T_e ($^{\circ}\text{C}$)</th><th>T_p ($^{\circ}\text{C}$)</th><th>T_e ($^{\circ}\text{C}$)</th><th>T_{p1} ($^{\circ}\text{C}$)</th><th>T_{p2} ($^{\circ}\text{C}$)</th><th>T_{p3} ($^{\circ}\text{C}$)</th></tr> <tr> <td>Crystals</td><td>129.3 \pm 0.8</td><td>132.0 \pm 0.3</td><td>199.0 \pm 0.4</td><td>228.7 \pm 0.3</td><td>236.2 \pm 0.1</td><td>238.1 \pm 0.2</td></tr> <tr> <td>Powder</td><td>130.1 \pm 0.6</td><td>131.9 \pm 0.2</td><td>199.3 \pm 0.3</td><td>227.1 \pm 0.6</td><td>235.6 \pm 0.3</td><td>238.0 \pm 0.2</td></tr> </table>						KDN type	Fusion (melting)		Decomposition				T_e ($^{\circ}\text{C}$)	T_p ($^{\circ}\text{C}$)	T_e ($^{\circ}\text{C}$)	T_{p1} ($^{\circ}\text{C}$)	T_{p2} ($^{\circ}\text{C}$)	T_{p3} ($^{\circ}\text{C}$)	Crystals	129.3 \pm 0.8	132.0 \pm 0.3	199.0 \pm 0.4	228.7 \pm 0.3	236.2 \pm 0.1	238.1 \pm 0.2	Powder	130.1 \pm 0.6	131.9 \pm 0.2	199.3 \pm 0.3	227.1 \pm 0.6	235.6 \pm 0.3	238.0 \pm 0.2
KDN type	Fusion (melting)		Decomposition																														
	T_e ($^{\circ}\text{C}$)	T_p ($^{\circ}\text{C}$)	T_e ($^{\circ}\text{C}$)	T_{p1} ($^{\circ}\text{C}$)	T_{p2} ($^{\circ}\text{C}$)	T_{p3} ($^{\circ}\text{C}$)																											
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Powder	130.1 \pm 0.6	131.9 \pm 0.2	199.3 \pm 0.3	227.1 \pm 0.6	235.6 \pm 0.3	238.0 \pm 0.2																											
ρ [g cm^{-3}]	2.206 ^[2] , 2.25 ^[6]																																
Heat of formation	-264.18 ± 0.54 kJ/mol ($\Delta_f H^{\circ}$) ^[1] , $-1,820.41 \pm 3.75$ kJ/kg ($\Delta_f H^{\circ}$) ^[1] , -63.14 kcal/mol ($\Delta H^{\circ}_{\text{f}}$, exptl.) ^[7] , -62.55 kcal/mol ($\Delta H^{\circ}_{\text{f}}$, calcd.) ^[7] , -63.14 ± 0.13 kcal/mol ($\Delta H^{\circ}_{\text{f}}$) ^[8]																																
	Calcd. (K-J)			Exptl.																													
$-\Delta_{\text{ex}} U^{\circ}$ [kJ kg $^{-1}$]																																	
T_{ex} [K]																																	
$p_{\text{C-J}}$ [GPa]																																	
VoD [m s^{-1}]																																	
V_0 [L kg $^{-1}$]																																	

5 s explosion T [°C] Ignition T [°C]	140 ^[6]															
Vacuum stability test [cm ³ /h]	22.9 mL/5 g @ 80 °C, 40 h ^[6]															
Thermal stability	<p>Overall mass loss = 35.6% (TG, N₂ atmosphere, two stage dec. process; 2.5% mass loss @ 70–110 °C and 33.1% >200 °C)^[9], overall mass loss = 30.2% (3 stage mass loss, TG @ 5 °C/min, Ar)^[9], TGA mass loss = 30.2%^[6]</p> <p>TG, 5 mg samples in Al crucibles with pinholes in lid, Ar, 10 °C/min^[9]:</p> <table><tr><th rowspan="2">KDN type</th><th colspan="3">Mass loss (%)</th></tr><tr><th>Stage 1 (occurs @ ~120 °C)</th><th>Stage 2 (main dec.)</th><th>Total</th></tr><tr><td>Crystals</td><td>0.46 ± 0.04</td><td>34.87 ± 0.14</td><td>35.33 ± 0.18</td></tr><tr><td>Powder</td><td>0.21 ± 0.01</td><td>34.90 ± 0.07</td><td>35.11 ± 0.06</td></tr></table>	KDN type	Mass loss (%)			Stage 1 (occurs @ ~120 °C)	Stage 2 (main dec.)	Total	Crystals	0.46 ± 0.04	34.87 ± 0.14	35.33 ± 0.18	Powder	0.21 ± 0.01	34.90 ± 0.07	35.11 ± 0.06
KDN type	Mass loss (%)															
	Stage 1 (occurs @ ~120 °C)	Stage 2 (main dec.)	Total													
Crystals	0.46 ± 0.04	34.87 ± 0.14	35.33 ± 0.18													
Powder	0.21 ± 0.01	34.90 ± 0.07	35.11 ± 0.06													
Solubility [g/mL]	Good solubility in water or MeOH but higher in water ^[12]															
Photosensitivity	Sensitive to daylight, after 24 h in daylight shows different DSC peak ^[9]															
$\Delta H^\circ_{\text{sol}}$ [kcal/mol]	11.28 ± 0.02 (H ₂ O) ^[8]															
Decomposition activation energy [kJ/mol]	142.9 ^[10]															

	KD ^N [4]	KD ^N [3]	KD ^N [3]	KD ^N [3]	KD ^N [3]	KD ^N [3]	KD ^N [3]
Chemical formula	KN ₃ O ₄	KN ₃ O ₄	KN ₃ O ₄	KN ₃ O ₄	KN ₃ O ₄	KN ₃ O ₄	KN ₃ O ₄
Molecular weight [g mol ⁻¹]	145.13	145.13	145.13	145.13	145.13	145.13	145.13
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	<i>P</i> 2 ₁ / <i>n</i> (no. 14)	<i>P</i> 2 ₁ / <i>n</i> (no. 14)	<i>P</i> 2 ₁ / <i>n</i> (no. 14)	<i>P</i> 2 ₁ / <i>n</i> (no. 14)	<i>P</i> 2 ₁ / <i>n</i> (no. 14)	<i>P</i> 2 ₁ / <i>n</i> (no. 14)	<i>P</i> 2 ₁ / <i>n</i> (no. 14)
<i>a</i> [Å]	6.614(1)	6.5891(4)	6.5918(4)	6.6010(3)	6.6029(4)	6.6114(1)	6.6162(2)
<i>b</i> [Å]	9.280(2)	9.0653(5)	9.0778(5)	9.1253(5)	9.1694(5)	9.2299(2)	9.2831(2)
<i>c</i> [Å]	7.198(1)	7.1459(4)	7.1540(4)	7.1657(4)	7.1731(4)	7.1878(2)	7.2000(3)
α [°]	90	90	90	90	90	90	90
β [°]	97.58(1)	97.975(2)	97.946(2)	97.890(1)	97.805(1)	97.639(1)	97.583(1)
γ [°]	90	90	90	90	90	90	90
<i>V</i> [Å ³]	437.94(13)	422.71(4)	423.98(4)	427.55(4)	430.27(4)	434.73(2)	438.35(2)
<i>Z</i>	4	4	4	4	4	4	4
ρ_{calc} [g cm ⁻³]	2.201	2.280	2.274	2.255	2.240	2.217	2.199
<i>T</i> [K]	296	85	100	150	200	250	298

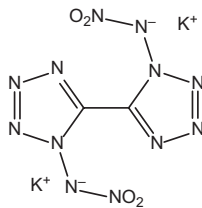
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Potassium 1,1'-dinitramino-5,5'-bistetrazolate

Name [German, acronym]: Potassium 1,1'-dinitramino-5,5'-bistetrazolate
[K2DNABT]

Main (potential) use: Primary explosive

Structural formula:



	K2DNABT	
Formula	C ₂ K ₂ N ₁₂ O ₄	
Molecular mass [g mol ⁻¹]	334.3	
Appearance at RT		
IS [J]	1 ^[1]	
FS [N]	<1 ^[1]	
ESD [J]	0.003 ^[1]	
N [%]	50.3	
Ω(CO ₂) [%]		
T _{dec.} [°C]	200 ^[1]	
ρ [g cm ⁻³]	2.11 (@ 298 K) ^[1]	
Heat of formation	326.4 kJ/mol (Δ _f H ^o _m) ^[1] , Δ _f U ^o = 1,036.1 kJ/kg (energy of form.) ^[1]	
	Calcd. (EXPLO5 6.02)	Exptl.
-Δ _{ex} U ^o [kJ kg ⁻¹]	4,959	
T _{ex} [K]	3,424	
p _{C-J} [kbar]	317	
VoD [m s ⁻¹]	8,330 (@ 2.11 g cm ⁻³)	
V ₀ [L kg ⁻¹]	489	

	K2DNABT^[1]
Chemical formula	C ₂ K ₂ N ₁₂ O ₄
Molecular weight [g mol ⁻¹]	334.3
Crystal system	Triclinic
Space group	<i>P</i> -1 (no. 2)
<i>a</i> [Å]	5.0963(6)
<i>b</i> [Å]	6.8248(8)
<i>c</i> [Å]	8.4271(8)
α [°]	7.56(1)
β [°]	86.15(1)
γ [°]	71.02(1)
<i>V</i> [Å ³]	225.65(5)
<i>Z</i>	1
ρ_{calc} [g cm ⁻³]	2.172
<i>T</i> [K]	100

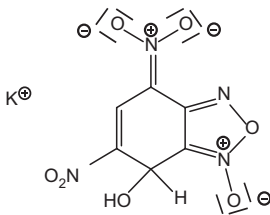
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Potassium dinitrobenzfuroxan

Name [German, acronym]: Potassium salt of 4,6-dinitrobenzfuroxan, 4,6-dinitrobenzofurazon-1-oxide potassium salt, potassium 4,6-dinitrobenzofurazan-1-oxide, potassium 4,6-dinitro-7-hydro-7-hydroxybenzfuroxamide [KDNBF]

Main (potential) use: Primary explosive^[1, 11], squibs, in primary compositions^[4], was used in low-toxicity mixtures for primer production^[14], “green” primary explosive alternative to LS in primer compositions^[15]

Structural formula:



	KDNBF																				
Formula	C ₆ H ₄ N ₄ O ₆ K																				
Molecular mass [g mol ⁻¹]	225																				
Appearance at RT	Orange-brown solid ^[1, 11] , small golden-orange plates ^[1] , red crystalline solid ^[4]																				
IS [J]	<p>3 in (1 lb mass, 7 mg sample)^[1], 7^[2], 3 in (2 kg mass, P.A.)^[11], same as LS^[14], <i>H</i>_{50%} = 35 cm (2 kg mass)^[13]</p> <p>Effect of liquid nitrogen on the IS (2 kg mass, modified P.A. machine, 50% point, <i>T</i> cycling = soaking sample in LN₂ for 15 min then allowing to stand at ambient <i>T</i> for 1 h for five cycles)^[17]:</p> <table><tr><td></td><td>Height (cm) (standard Deviation)</td></tr><tr><td colspan="2">Mean height for 50% probability of reaction</td></tr><tr><td>Control (dry)</td><td>27.31 (1.24)</td></tr><tr><td>LN₂ test</td><td>27.61 (4.24)</td></tr><tr><td colspan="2">Height for 10% probability of reaction</td></tr><tr><td>Control (dry)</td><td>5.08</td></tr><tr><td>LN₂ test</td><td>12.50</td></tr><tr><td colspan="2">Effect of <i>T</i> cycling at 50% height</td></tr><tr><td>In LN₂, % fire</td><td>75</td></tr><tr><td>Dry, % fire</td><td>60</td></tr></table>		Height (cm) (standard Deviation)	Mean height for 50% probability of reaction		Control (dry)	27.31 (1.24)	LN ₂ test	27.61 (4.24)	Height for 10% probability of reaction		Control (dry)	5.08	LN ₂ test	12.50	Effect of <i>T</i> cycling at 50% height		In LN ₂ , % fire	75	Dry, % fire	60
	Height (cm) (standard Deviation)																				
Mean height for 50% probability of reaction																					
Control (dry)	27.31 (1.24)																				
LN ₂ test	27.61 (4.24)																				
Height for 10% probability of reaction																					
Control (dry)	5.08																				
LN ₂ test	12.50																				
Effect of <i>T</i> cycling at 50% height																					
In LN ₂ , % fire	75																				
Dry, % fire	60																				

FS [N]	38 ^[2] , same as LS ^[14] , explodes with steel shoe (friction pendulum test) ^[1, 4] , explodes with fiber shoe (friction pendulum test) ^[1, 4] , $F_{50\%} = 400 \pm 100$ g (Julius-Peters, BAM, porcelain plate and peg, Bruceton method) ^[12] , $F_{10\%} = 50$ g (Julius-Peters, BAM, porcelain plate and peg, Bruceton method) ^[12] , insensitive up to 3.8 kg (Julius-Peters apparatus) ^[13]	
ESD [J]	fires @ 4.5, 0.45 and 0.045 ^[5]	
N [%]	19.9	
$\Omega(\text{CO}_2)$ [%]		
$T_{\text{m.p.}}$ [°C]	215 ^[2] , explodes @ 210 ^[1, 6] , 215 (melts with dec., onset, hot-stage microscopy @ 10 °C/min) ^[5] , 210 ^[11] , 215 (explodes) ^[13] , 222 (exo, DTA @ 10 °C/min, static air) ^[13]	
$T_{\text{dec.}}$ [°C]	210 (onset, DTA) ^[4] , 224.5 (peak max., exotherm, @ 10 °C/min) ^[5] , 217 (DSC) ^[10] , 210 (dec., explosive) ^[4] , 190 (onset for intensive dec.) ^[14] , 217 ^[15] , 203 (DTA/TGA) ^[16]	
ρ [g cm ⁻³]	2.21 ^[1, 4] , 2.21 (crystal) ^[14] , Loading density (g cm ⁻³ @ psi $\times 10^3$) ^[1] : 1.63 @ 10 ^[1] , 1.77 @ 20 ^[1] , 1.81 @ 30 ^[1] , 1.86 @ 40 ^[1] , 1.98 @ 80 ^[1]	
Heat of formation		
Heat of combustion	2,209 kcal/kg ^[1, 7]	
	Calcd. (EXPLO5 6.03)	Exptl.
$-\Delta_{\text{ex}}U^\circ$ [kJ kg ⁻¹]		725 cal/g ^[1, 7]
T_{ex} [K]		
$p_{\text{c-j}}$ [kbar]		
VoD [m s ⁻¹]		
V_0 [L kg ⁻¹]		604 ^[1]

Sand test [g]	93% TNT ^[4, 8] , 44.8 g ^[4] , 43.6–44.8 g (200 g bomb) ^[11]
Initiation efficiency	0.30 g MF or 0.10 g LA minimum charges required for initiation ^[4] , lower initiation ability than that of MF ^[14]
5 s explosion T [°C] 5 s ignition T [°C]	250 ^[1, 11] 250 ^[7]
Ignition T [°C] Explosion T [°C]	199, 200, 201 (50 mg sample, @ 5 °C/min) ^[5] , ~210 ^[14] 210 (explosive dec.) ^[4]
Autoignition T [K]	453 ^[12]
100 °C heat test [% mass loss]	0.03% mass loss in first 48 h ^[1, 4] , 0.05% mass loss in second 48 h ^[1, 4] , no explosions in 100 h ^[1, 4] , <0.1% mass loss @ 100 °C for 4 days ^[11]

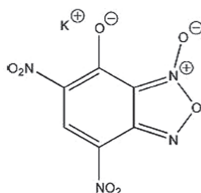
Thermal stability	Main exo dec. peak shifts from 203 °C to 177 °C (DTA/TGA) after two sterilization cycles at 125 °C for 64 h each ^[16] , no change in morphology of crystals after two sterilization cycles (@ 125 °C for 64 h each) ^[16] , 0.55 mg (1.32%) weight loss over 255 day test period in accelerated aging test (equivalent to 8.5 years) ^[16] , DTA/TGA after 183 days accelerated aging equivalent to 6.1 years) shows no significant changes ^[16]																																	
Solubility [g/mL]	0.245 g/100 g H ₂ O @ 30 °C ^[1, 4] ,																																	
Hygroscopicity	0.11% @ 30 °C with 75% RH ^[1] , 0.27% @ 30 °C with 90% RH ^[1, 4] , only slightly hygroscopic ^[11]																																	
Blast wave characteristics	Blast wave overpressure P_{\max} = 4.1 kPa (mean value) ^[9] , blast wave positive phase impulse I^+ = 0.56 Pa s (mean value) ^[9] (loose filled into mild steel test units (4.6 × 2.5 × 2.5 cm, 0.9 cm hole diameter) sealed with a cork disc and adhesive mass of material = 200–1,000 mg, initiated with an ICI type “E” fusehead) ^[9]																																	
Specific heat [cal/g/°C]	0.217 @ –50 °C ^[1] , 0.217 @ 0 °C ^[1] , 0.217 @ 25 °C ^[1] , 0.217 @ 50 °C ^[1, 4]																																	
Stab sensitivity	Stab sensitivity values from ^[1] : <table><tr><th rowspan="2">Density (g/cc)</th><th colspan="3">Firing point (inch-ounces)</th></tr><tr><th>0%</th><th>50%</th><th>100%</th></tr><tr><td>1.63</td><td>73</td><td>79</td><td>84</td></tr><tr><td>1.77</td><td>66</td><td>75</td><td>83</td></tr><tr><td>1.81</td><td>42</td><td>48</td><td>64</td></tr><tr><td>1.86</td><td>12</td><td>15</td><td>18</td></tr><tr><td>1.93</td><td>11</td><td>17</td><td>21</td></tr><tr><td>1.98</td><td>7</td><td>11</td><td>14</td></tr></table>			Density (g/cc)	Firing point (inch-ounces)			0%	50%	100%	1.63	73	79	84	1.77	66	75	83	1.81	42	48	64	1.86	12	15	18	1.93	11	17	21	1.98	7	11	14
Density (g/cc)	Firing point (inch-ounces)																																	
	0%	50%	100%																															
1.63	73	79	84																															
1.77	66	75	83																															
1.81	42	48	64																															
1.86	12	15	18																															
1.93	11	17	21																															
1.98	7	11	14																															

Radiation sensitivity	Effects of reactor irradiation, ^a average reactor exposure rates: fast neutrons $\phi > 0.18 \text{ MeV } 1.4 \times 10^{13} \text{ n/cm}^2 \text{ s}$, thermal neutron $\phi > 0.17 \text{ eV } 8.6 \times 10^{13} \text{ n/cm}^2 \text{ s}$, gamma $4.0 \times 10^8 \text{ R/h}$ ($3.38 \times 10^{10} \text{ ergs/g (C)/h gamma}$), ^b sample detonated, ^c 200 °C ^[18] .								
	Irradiation time (min)	Total neutron dose		Total gamma (R)	Weight loss (%)	10% loss on TGA (°C)	150° avg. gas evolution (mL/g/h)	DTA peak exotherm @ 20 °C/min (°C)	5 s explosion T (°C)
		Fast (n/cm ²)	Thermal (n/cm ²)						
	0					210	2.55	212 ^b	194
	60	5.04×10^{16}	3.10×10^{17}	4.0×10^8	0.46	188	10.95	198 ^b	185
	120	1.01×10^{17}	6.19×10^{17}	8.0×10^8	1.52	188	11.0	188 ^b	170
	180	1.61×10^{17}	9.29×10^{17}	1.2×10^9	4.84 ^c	175	11.0	182 ^b	169

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Potassium 5,7-dinitro-[2,1,3]-benzoxadiazol-4-olate 3-oxide

- Name [German, acronym]: Potassium 5,7-dinitro-[2,1,3]-benzoxadiazol-4-olate-3-oxide, potassium 4,6-dinitro-7-hydroxybenzofuroxan, 4,6-dinitro-7-hydroxybenzofuroxan, potassium salt [KDNP]
- Main (potential) use: Primary explosive, possible LS replacement^[3], tests for use in percussion primers, impulse cartridges and other initiators^[3], fast deflagrating material^[6], evaluated for use in a bridgewire slurry mix in CCU-63 impulse cartridge^[6], evaluated for use in TOW missile initiator units pressed onto bridgewire^[6], evaluated for use as a component of a primer mix in PVU-12/A percussion primers^[6, 7], green replacement for LS (patent pending)^[6], lead-free replacements for primers^[7]
- Structural formula:



	KDNP
Formula	C ₆ HN ₄ O ₇ K
Molecular mass [g mol ⁻¹]	280.21
Appearance at RT	Light brown solid/crystalline solid ^[1]
IS [J]	0.05 ^[1] , 51 mJ (ball drop, needles) ^[2] , 0.047 ^[5] , 0.047 ± 0.004 (ball drop apparatus, 50% value) ^[1]
FS [N]	10 ^[1] , 175 g no-fire level, 200 g low-fire level (BAM, needles) ^[2] , 9.81 ^[5] , 9.81 (no fire, Julius-Peters small BAM) ^[1] , 10.79 (low-fire, Julius-Peters small BAM) ^[1]
ESD [J]	>2 mJ ^[1] , >675 μJ ^[5] , <675 μJ (no fire, confined, LEESA or Electro-Tech systems model 931) ^[1] , >675 μJ (low fire, confined, LEESA or Electro-Tech systems model 931) ^[1] , >1.88 mJ (no-fire, unconfined, LEESA or Electro-Tech systems model 931) ^[1]
N [%]	20.0 ^[1]
Ω(CO ₂) [%]	
T _{m,p.} [°C]	Explodes @ 350 ^[1]

$T_{\text{dec.}}$ [°C]	350 (explodes) ^[1] , 278 (onset, DSC @ 20 °C/min) ^[2] , ~270 (onset of intensive dec., DSC) ^[4] , ~285 (DSC) ^[3] , 284.57 (exo peak max., DSC @ 20 K/min, 1 mg sample, sealed Al cup, Ar) ^[1] , 285 ^[5]		
ρ [g cm ⁻³]	1.982 (@ 103 K) ^[1] , 1.945 (@ 298 K), 1.94–2.13 (anhydrous salt) ^[2] , 1.982 (crystalline) ^[5]		
Heat of formation	–197.07 kJ/mol ($\Delta_f H^\circ$, bomb calorimetry) ^[1] , 197.07 kJ/mol ($\Delta_f H^\circ$) ^[5]		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{\text{ex}} U^\circ$ [kJ kg ⁻¹]	4,757	3,280 ^[5]	3,280 (bomb calorimetry) ^[1]
T_{ex} [K]	3,453		
$p_{\text{C-J}}$ [kbar]	242		
VoD [m s ⁻¹]	7,486 (@ 1.945 g cm ⁻³)		
V_0 [L kg ⁻¹]	467		

Critical T [°C]	483–503 K (1 cm diameter sphere @ 80% TMD) ^[1]		
5 s explosion T [°C]	562 K (deflagration) ^[1]		
1 s explosion T [°C]	573 K (deflagration) ^[1]		
10 s explosion T [°C]	557 K (deflagration) ^[1]		
Thermal stability	≤1% mass loss (mainly surface water loss, TGA, isothermally @ 393 K, Al, @ 5 K/min up to 393 K then maintained for 90 h @ 393 K, Ar, Alumina pans) ^[1] , ~6% mass loss (rapid mass loss during heating if KDNP prepared or recryst. from H ₂ O, TGA, isothermally @ 393 K, Al, @ 5 K/min up to 393 K then maintained for 90 h @ 393 K, Ar, Alumina pans) ^[1]		
Solubility [g/mL]	Can be recryst. from acetone/toluene ^[1] , soluble in 2-methoxyethanol ^[1]		
Hygroscopicity	Rel. nonhygroscopic gains 1–2% surface water over time ^[1]		
	Values from ^[1] :		
	Rel. humidity (%)	T (K)	Time (h)
	92	293	24
	92	293	48
	55	293	35 days
Compatibility	Compatible with 1100 aluminum, 6061-T6 aluminum, 2024-T3 aluminum, 304 stainless steel, brass, Tophet C (Nichrome), Tophet A, EvenOhm, BKNO ₃ , FFG black powder, red Dor, Hi-Temp ^[1]		

Thermal conductivity	0.09 W m ⁻¹ K ⁻¹ (@ 303 K, for free flowing cryst. powder) ^[1]																				
pK _a	pH = 5.35 (0.45 g KDNP in 100 mL deionized water) ^[1]																				
Closed bomb data	T ₀ = application of pulse, T _{p0} = time to first indication of pressure, T _{pk} = time-to-peak pressure, * = first perturbation in current or voltage trace, data from ^[7] : <table><tr><td>T₀-T_{p0}</td><td>T₀-T_{pk}</td><td>T_{p0}-T_{pk}</td><td>Ignition time *(ms)</td><td>Peak pressure (psi)</td><td>Charge weight (g)</td><td>Impetus (in lb/g)</td></tr><tr><td>0.781</td><td>0.913</td><td>0.132</td><td>0.710</td><td>1,480</td><td>0.149</td><td>6,047</td></tr></table>							T ₀ -T _{p0}	T ₀ -T _{pk}	T _{p0} -T _{pk}	Ignition time *(ms)	Peak pressure (psi)	Charge weight (g)	Impetus (in lb/g)	0.781	0.913	0.132	0.710	1,480	0.149	6,047
T ₀ -T _{p0}	T ₀ -T _{pk}	T _{p0} -T _{pk}	Ignition time *(ms)	Peak pressure (psi)	Charge weight (g)	Impetus (in lb/g)															
0.781	0.913	0.132	0.710	1,480	0.149	6,047															

	KDNP^[1]
Chemical formula	C ₆ HKN ₄ O ₇
Molecular weight [g mol ⁻¹]	280.21
Crystal system	Monoclinic
Space group	$P2_1/c$ (no. 14)
a [Å]	7.4789(7)
b [Å]	9.8999(9)
c [Å]	12.8390(11)
α [°]	90
β [°]	98.945(2)
γ [°]	90
V [Å ³]	939.04(15)
Z	4
ρ_{calc} [g cm ⁻³]	1.982 (@ 103 K) 1.945 (@ 298 K)
T [K]	103 K

- [1] J. F. Fronabarger, M. D. Williams, W. B. Sanborn, D. A. Parrish, M. Bichay, *Propellants, Explosives, Pyrotechnics*, **2011**, 36, 459–470.
- [2] R. Matyáš, J. Pachman, *Primary Explosives*, Springer-Verlag, **2013**, pp. 176–179.
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- [5] J. J. Sabatini, K. D. Oyler, *Crystals*, **2016**, 6, 5.
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- [7] J. W. Fronabarger, M. D. Williams, *Lead-Free Primers*, US Patent 2012/0152140 A1, June 21st **2012**.

Potassium nitrate

Name [German, acronym]: Potassium nitrate, niter^[17], nitre^[17], nitrate of potash, sal prunella (KNO₃ that has been melted and cast into blocks)^[17] [kaliumnitrat, salpeter, kalisalpeter]

Main (potential) use: Pyrotechnical compositions, manufacture of fuses, matches, component of propellants, ingredient in black powder – not an explosive^[15], naturally occurring pyrotechnic oxidizer^[17]

Structural formula:



	Potassium nitrate
Formula	KNO ₃
Molecular mass [g mol ⁻¹]	101.1
Appearance at RT	White powder ^[15] , colorless crystals/white powder ^[17] , colorless, transparent prisms, white granular or crystalline powder ^[18]
N [%]	13.86
Ω(CO ₂) [%]	+39.6
T _{phase transition} [°C]	~128 (α-KNO ₃ (orthorhombic) → β-KNO ₃ (trigonal)) ^[6] , cooling β-KNO ₃ from 200 °C passes through γ-KNO ₃ (trigonal) before reverting to α-KNO ₃ @ 100 °C ^[6] , 114–139 (endotherm), 128 (rhombic → trigonal, DTA @ 15 °C/min) ^[7] , 137 (endo, onset), 145 (endo peak max) (DSC @ 20 °C/min) ^[14]
T _{m.p.} [°C]	330 ^[1] , 314 ^[5, 17] , 333 ^[18] , 322 (fusion, DSC @ 20 °C/min) ^[14]
T _{dec.} [°C]	340 (DTA) ^[1] , 332 (fusion), 628 (slight bubbling), 642 (rapid bubbling), 805 (slight nitrous fumes) ^[7] , no exothermic peak <450 °C (DSC @ 20 °C/min) ^[14] , ~600–750 °C (dec. forming KNO ₂ and O ₂) ^[17] , >800 °C (dec. forming K ₂ O, KO ₂ , K ₂ O, O ₂ and NO _x) ^[17] , 400 ^[18]

ρ [g cm ⁻³]	2.1 (@ 298 K) ^[2] , 2.123 ^[4] , 2.10 ^[5, 17] , 2.1062–2.109 (crystal) ^[11] , 2.11 ^[18]	
Heat of formation	–4,891 kJ/kg (enthalpy of form.) ^[5] , –1,167 cal/g ^[4] , –117.76 kcal/mol (ΔH_f°) ^[13] , 117.7 kcal/mol (ΔH_f° , exptl.) ^[12] , 116.7 kcal/mol (ΔH_f° , calcd.) ^[12] , –495 kJ/mol (enthalpy of form.) ^[17]	
	Calcd. (EXPLO5 6.04)	Exptl.
$-\Delta_{\text{ex}}U^\circ$ [kJ kg ⁻¹]		
T_{ex} [K]		
$p_{\text{C-J}}$ [kbar]		
VoD [m s ⁻¹]		
V_0 [L kg ⁻¹]		

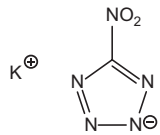
Solubility [g/mL]	Soluble in cold H ₂ O ^[15] , very soluble in hot water ^[15] , insoluble in EtOH and Et ₂ O ^[15] , 38 g/100 g in H ₂ O @ 25 °C ^[17] , insoluble in EtOH ^[17] , 1 g in 2.8 mL H ₂ O ^[18] , 1 g/0.5 mL boiling H ₂ O ^[18] , 1 g/620 mL EtOH ^[18] , soluble in glycerol ^[18] , insoluble in abs. alcohol ^[18] , dissolves in H ₂ O with lowering of temperature ^[18]
Hygroscopicity	Critical humidity = 94.2% RH @ 20 °C ^[16, 17]
Compatibility	Should not be mixed with AP ^[17] , mixture with red phosphorus is highly impact sensitive ^[17] , mixtures with combustible dust are dangerous ^[17] , can burn for hours with combustible substances ^[17] , incompatible for long-term storage with Al under moist conditions ^[17]
Enthalpy of dec. [kJ/mol]	225 (for dec. to KNO ₂) ^[17] , 188 (for dec. to K ₂ O, N ₂ and O ₂) ^[17]
pH	~7 ^[18]

	KNO_3 [8]	KNO_3 [9]	KNO_3 [9]	KNO_3 [10]	KNO_3 [9]	KNO_3 [9]	KNO_3 [3]	KNO_3 [3]
	$\alpha\text{-KNO}_3$	$\beta\text{-KNO}_3$ (powder)	$\gamma\text{-KNO}_3$ (powder)	$\delta\text{-KNO}_3$	High pressure phase	$\gamma\text{-KNO}_3$ (Phase-II)	$\gamma\text{-KNO}_3$ (Phase-III)	
Chemical formula	KNO_3	KNO_3	KNO_3	KNO_3	KNO_3	KNO_3	KNO_3	KNO_3
Molecular weight [g mol ⁻¹]	101.11	101.11	101.11	101.11	101.11	101.11	101.11	101.11
Crystal system	Orthorhombic	Hexagonal	Hexagonal	Monoclinic	Orthorhombic	Hexagonal	Hexagonal	Hexagonal
Space group	$Pm\bar{c}n$	$R\bar{3}m$ (no. 166)	$R\bar{3}m$ (no. 160)	$P2_1/c$ (no. 14)	$Pnm\bar{a}$ (no. 62)	$R\bar{3}m$ (no. 160)	$R\bar{3}m$ (no. 160)	$R\bar{3}m$ (no. 160)
a [Å]	5.414(2)	5.425(1)	5.487(1)	3.6820(7)	7.4867(2)	5.4698(8)	5.4325(2)	5.4325(2)
b [Å]	9.166(9)	5.415(1)	5.487(1)	5.5830(11)	5.5648(2)	5.4698(8)	5.4325(2)	5.4325(2)
c [Å]	6.431(9)	9.386(4)	9.156(3)	15.065(3)	6.7629(2)	8.992(3)	8.8255(7)	8.8255(7)
α [°]	90			90	90			
β [°]	90			103.91(3)	90			
γ [°]	90			90	90			
V [Å ³]				300.6	281.76	232.99(8)	225.56(2)	225.56(2)
Z	4	3	3	4		3	3	3
ρ_{calc} [g cm ⁻³]				2.23				
T [K]	25 °C	151 °C	91 °C	293		295	123	

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- [5] R. Meyer, J. Köhler, A. Homburg, *Explosives*, 7th edn., Wiley-VCH, Weinheim, **2016**, p. 268.
- [6] J. K. Nimmo, B. W. Lucas, *Acta Cryst.*, **1976**, B32, 1968–1971.
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- [17] K. L. Kosanke, B. J. Kosanke, B. T. Sturman, R. M. Winokur, *Encyclopedic Dictionary of Pyrotechnics (and Related Subjects), Part 3 – P to Z*, Pyrotechnic Reference Series No.5, Journal of Pyrotechnics Inc., Whitewater, Colorado, USA, **2012**, pp. 859–862.
- [18] *The Merck Index – An Encyclopedia of Chemicals and Drugs*, 9th edn., M. Windholz, S. Budavari, L. Y. Stroumstos, M. N. Fertig (eds.), Merck and Co. Inc., Rahway, New Jersey, USA, **1976**.

Potassium 5-nitrotetrazolate

Name [German, acronym]: Potassium nitrotetrazolate, [kalium 5-nitrotetazolat]
Main (potential) use: Potential green primary explosive^[2]
Structural formula:



	Potassium 5-nitrotetrazolate		
Formula	CKN ₅ O ₂		
Molecular mass [g mol ⁻¹]	153.14		
Appearance at RT			
IS [J]	10 (BAM) ^[1] , 10 ^[2]		
FS [N]	<5 (BAM) ^[1] , <5 ^[2]		
ESD [J]			
N [%]	45.73		
Ω(CO ₂) [%]			
T _{m,p.} [°C]	168 (onset, DSC @ 5 °C/min) ^[1] , 168 ^[2]		
T _{dec.} [°C]	195 (DSC @ 5 °C/min) ^[1, 2]		
ρ [g cm ⁻³]	2.027 (X-ray @ 200 K) ^[1, 2]		
Heat of formation			
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
−Δ _{ex} U° [kJ kg ⁻¹]			
T _{ex} [K]			
p _{C-J} [kbar]			
VoD [m s ⁻¹]			
V ₀ [L kg ⁻¹]			
Solubility [g/mL]	Soluble in H ₂ O, MeOH, acetone, DMSO ^[1]		
Flame sensitivity	Explodes ^[1, 2]		

	KNT^[1]
Chemical formula	CKN ₅ O ₂
Molecular weight [g mol ⁻¹]	153.16
Crystal system	Monoclinic
Space group	<i>P</i> 2 ₁ / <i>c</i>
<i>a</i> [Å]	4.8268(3)
<i>b</i> [Å]	13.1717(8)
<i>c</i> [Å]	7.9423(6)
α [°]	90
β [°]	96.363(7)
γ [°]	90
<i>V</i> [Å ³]	501.84(6)
<i>Z</i>	4
ρ_{calc} [g cm ⁻³]	2.027
<i>T</i> [K]	200
	Crystals from slow evaporation of MeOH soln.

[1] T. M. Klapötke, C. M. Sabaté, J. M. Welch, *Dalton Trans.*, **2008**, 6372–6380.

[2] M. A. Ilyushin, I. V. Tselinsky, I. V. Shugalei, *Centr. Eur. J. Energet. Mater.*, **2012**, 9, 293–327.

Potassium perchlorate

Name [German, acronym]: Potassium perchlorate, peroidin [kaliumperchlorat]
Main (potential) use: Pyrotechnics, oxidant in pyrotechnic compositions^[10],
common oxidizer in pyrotechnics^[12]
Structural formula: KClO_4

	Potassium perchlorate	
Formula	KClO_4	
Molecular mass [g mol ⁻¹]	138.6	
Appearance at RT	White rhombohedral cryst. solid ^[4] , colorless crystals/white powder ^[12, 13]	
IS [J]	Insensitive, that is, $H_{50\%} > 320$ cm (2.5 kg mass) ^[4] , mixtures with 1% ferric oxide, Mn dioxide, sugar, ammonium dichromate and 50/50 mixture with AN all insensitive (2.5 kg mass, > 320 cm) ^[4]	
N [%]	±0	
Ω(CO ₂) [%]	+46.2 (K ₂ O, HCl)	
T _{phase transition} [°C]	300 (rhombohedral → cubic) ^[4, 5] , 284–301 (endotherm, DTA transition $T = 300$ °C, rhombic → cubic, DTA @ 15 °C/min) ^[5] , 300 (crystal phase transition) ^[10]	
T _{m,p.} [°C]	525 ^[1, 4] , 588 (with dec.) ^[4] , 588 (fusion, DTA @ 15 °C/min) ^[5]	
T _{dec.} [°C]	510 ^[4] , 530 ^[4] , 588 (fusion), 619 (rapid bubbling), 616 (vigorous bubbling) (DTA @ 15 °C/min) ^[5] , 600 ^[6] , 653 ^[10] , 400 ^[13]	
ρ [g cm ⁻³]	2.53 ^[1] , 2.519 ^[3] , 2.530 (@ 25 °C) ^[4] , 2.5374 (@ 0 °C) ^[4] , sp. gr. = 2.53 g/mL ^[10] , 2.52 ^[12, 13] , 2.53574 ± 0.0001 @ 0 °C ^[4]	
Heat of formation	−111.29 kcal/mol (Q_f) ^[4] , −742 cal/g ^[3] , −103.22 kcal/mol (ΔH_f) ^[6] , −103.37 kcal/mol (ΔH°_f , exptl.) ^[8] , −101.07 kcal/mol (ΔH°_f , calcd.) ^[8] , −433 kJ/mol (enthalpy of form.) ^[12]	
	Calcd. (EXPLO5 6.03)	Exptl.
−Δ _{ex} U° [kJ kg ⁻¹]		
T _{ex} [K]		
p _{C-J} [kbar]		
VoD [m s ⁻¹]		
V ₀ [L kg ⁻¹]		

5 s explosion T [°C] Explosion T [°C]	240 (80/20 mixture with ethylene glycol) ^[4] , 290 (80/20 mixture with polyester resin) ^[4] , 245 (80/20 mixture with cotton linters) ^[4]		
Burn rate [mm/s]	Catalysis of burning rate of stoichiometric aluminum-potassium chlorate mixtures ^[6] :		
	Additive	Weight, %	Burning rate in s^{-1} at 100 psi
	None		0.38
	Chlorium dioxide	10	0.70
	Cobaltic oxide	10	0.80
	Ferric oxide	10	0.93
	Manganese dioxide	10	0.89
	Nickel oxide	10	0.70
	Cobalt chromate	10	1.15
	Cobalt	10	0.87
	Copper	10	0.74
	Lead	13	0.90
	Tin	6	0.94
	Ferrovandium	10	0.63
Flame T	$T = 3,024$ K (100 psi), S.I. = 206.5 lb s^{-1} lb (stoichiometric combustion with high grade paraffin as fuel, $(CH_2)_n$ and $\Delta H_f = -5.971$ kcal/mol @ 298 K) ^[6]		
Solubility [g/mL]	0.11 g/100 g MeOH ^[6] , 0.02 g/100 g EtOH ^[6] , 0.01 g/100 g <i>n</i> -propanol ^[6] , 0.005 g/100 g <i>n</i> -butanol ^[6] , 0.16 g/100 g acetone ^[6] , insoluble in Et ₂ O ^[6] , 0.7 parts KClO ₄ per 100 parts H ₂ O @ 0 °C ^[7] , 18.7 parts KClO ₄ per 100 parts H ₂ O @ 100 °C ^[7] , 2.1 g/100 g H ₂ O @ 25 °C ^[12] , soluble in 65 parts cold water ^[13] , soluble in 15 parts boiling water ^[13] , practically insoluble in EtOH ^[13] , 0.75 g/100 g H ₂ O @ 0 °C ^[4] , 18.2 g/100 g H ₂ O @ 100 °C ^[4] , 70 g/100 g H ₂ O @ 265 °C ^[4]		
Hygroscopicity	Critical humidity = 99.8% RH @ 15 °C ^[11] , not hygroscopic ^[12]		

Compatibility

Relative catalytic activity of metal oxides with potassium perchlorate as shown by DTA and TGA data from^[6]:

Catalyst	<i>T</i> of initial dec. (°C)	Catalyst	<i>T</i> of initial dec. (°C)
None	600	MnO ₂	460
ZnO	565	Fe ₂ O ₃	450
TiO ₂	535	CuO	450
Al ₂ O ₃	530	CoO	380
MgO	525	Cu ₂ O	380
NiO	520	Co ₃ O ₄	375
Ag ₂ O	520	Cr ₂ O ₃	325

Oxidation of fuels by potassium perchlorate, data from^[6]:

Fuel	<i>T</i> (°C)	Catalysts	Inhibitors	Comments
Carbon black	320–385			No induction period
Nuchar sugar charcoal		Alkali and alkaline earth halides	Basic salts	CO ₂ only gaseous product
Carbon black	343	LiCl, BaCl ₂ , KCl, NaCl	KI, Li ₂ CO ₃	
Synthetic diamond	380	V ₂ O ₅ , Fe ₂ (SO ₄) ₃ , Al ₂ (SO ₄) ₃ , Cu, Al	–	V ₂ O ₅ catalyst
Graphite	380	V ₂ O ₅	–	Sandwich tablets also studied
Toluene, Naphthalene,	370–440	–	–	No reaction
Anthracene	510	–	–	Explosion
Decalin, Cyclohexane, Cyclohexanol, Cyclohexanone	350–380	–	–	Dehydrogenation

	Polystyrene	300–550	–	–	No reaction
	Styrene copolymer	360–400	LiCl	K ₂ CO ₃ no effect	
	Bakelite	367	LiCl → ignition in 2–3 min	K ₂ CO ₃ inhibited	15% reaction in 5 h with no additive
	Novolac	367	LiCl → ignition at 355 °C K ₂ CO ₃ → ignition at 367 °C	–	30% reaction in 5 h with no additive
	Alicyclic compounds	–	–	–	Chromic oxide, BaO ₂ , PbO ₂ had no effect
	Polydivinylbenzene (PDVB)	400	O ₂ , air, CO ₂	–	Air at various pressures
	PDVB	420–490	V ₂ O ₅ and wide range of compounds	Li ₂ CO ₃ , Zn, Pb ₃ O ₄ , Al, Cu, Fe	From ignition delays decomposition at 360° gave a similar division
	PDVB	275–350	–	–	Sodium perchlorate as oxidizer
Forms sensitive mixtures with red phosphorus, arsenic sulfide and antimony sulfide and sulfur ^[12] , dec. promoted by KCl, FeCl ₃ , CuCl ₂ , Cr ₂ O ₃ , K ₂ Cr ₂ O ₇ and LiCl ^[12]					
$\Delta H^\circ_{\text{sol}}$ [kcal/mol]	12.20 ± 0.05 ^[9] , 12.335 ± 0.010 ^[9]				
Enthalpy of decomposition [kJ/mol]	–4 ^[12]				

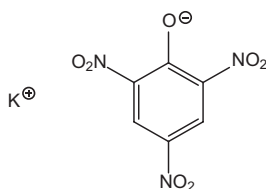
	Potassium perchlorate ^[2]
Chemical formula	KClO ₄
Molecular weight [g mol ⁻¹]	138.55
Crystal system	Orthorhombic
Space group	<i>Pnma</i>
<i>a</i> [Å]	8.7684(3)
<i>b</i> [Å]	5.6237(2)
<i>c</i> [Å]	7.2039(3)
α [°]	90.0
β [°]	90.0
γ [°]	90.0
<i>V</i> [Å ³]	355.23(2)
<i>Z</i>	4
ρ_{calc} [g cm ⁻³]	2.591
<i>T</i> [K]	126

- [1] “Hazardous Substances Data Bank” data were obtained from the National Library of Medicine (US)
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- [3] <https://engineering.purdue.edu/~propulsi/propulsion/comb/propellants.html>
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- [9] Y. N. Matyushin, T. S. Kon'kova, *To A Question on the Enthalpy of Formation of the Ammonium Perchlorate*, ICT **2003**, Karlsruhe, Germany, pp. 121-1–121-14.
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- [12] K. L. Kosanke, B. J. Kosanke, B. T. Sturman, R. M. Winokur, *Encyclopedic Dictionary of Pyrotechnics (and Related Subjects), Part 3 – P to Z*, Pyrotechnic Reference Series No.5, Journal of Pyrotechnics Inc., Whitewater, Colorado, USA, **2012**, pp. 862–864.
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Potassium picrate

- Name [German, acronym]:** Potassium salt of 2,4,6-trinitrophenol, potassium 2,4,6-trinitrophenolate, potassium 2,4,6-trinitrophenate, potassium salt of picric acid, potassium 2,4,6-trinitrophenoxide [kaliumpikrat, PP]
- Main (potential) use:** Was used in the past as a component of high explosives and smokeless powders^[2] formerly the principal ingredient in pyrotechnic whistle compositions^[2], mixtures with PETN or HMX can be used as initiators of other explosives charges in low-voltage detonators containing no primary explosives^[8], was used in the explosives poudres Designolles and poudres Fontaine^[14], in pyrotechnic whistle compositions, propellants such as Ballistite, some primer mixtures^[14]

Structural formula:



	Potassium picrate
Formula	$\text{C}_6\text{H}_2\text{KN}_3\text{O}_7$
Molecular mass [g mol ⁻¹]	267.19
Appearance at RT	Reddish-yellow crystalline solid ^[2] , crystals range in color from yellow to deep orange/red-brown with the darker colors suggested to be an impurity produced by overheating the salt soln. in an excess of base, the orange gave the same X-ray diffraction pattern as the yellow crystals ^[10] , yellow needle crystals (pure) ^[10] , long thin yellow crystals from aqueous soln. ^[4] , reddish or yellow rhombic crystals ^[14]
IS [J]	125 cm (detonates, air-dry sample, 750 g mass) ^[7] , $H_{50} = 37.3 \pm 0.05$ cm (type 12, ERL apparatus) ^[13] , $H_{50} = 55.9 \pm 0.04$ cm (type 12B, ERL apparatus) ^[13]

ESD [J]	Data from ^[9] : <table><tr><th colspan="3">50% point energy (J)</th></tr><tr><td>3 mil foil</td><td>10 mil foil</td><td>% expl.</td></tr><tr><td>0.73</td><td>0.54</td><td>100</td></tr></table> Data form ^[13] : <table><tr><th colspan="2">Energy (J)</th></tr><tr><td>0.076 mm foil</td><td>0.254 mm foil</td></tr><tr><td>0.73</td><td>0.54</td></tr></table>			50% point energy (J)			3 mil foil	10 mil foil	% expl.	0.73	0.54	100	Energy (J)		0.076 mm foil	0.254 mm foil	0.73	0.54
50% point energy (J)																		
3 mil foil	10 mil foil	% expl.																
0.73	0.54	100																
Energy (J)																		
0.076 mm foil	0.254 mm foil																	
0.73	0.54																	
N [%]	15.73																	
Ω(CO ₂) [%]																		
T _{m.p.} [°C]	Melts before it violently decomposes ^[14]																	
T _{phase transition} [°C]	3 polymorphs reported (A, B and C): type A obtained when an aqueous/ alcohol soln. of PA is neutralized with KOH soln.; type B obtained on using methylated at RT or isopropyl alcohol or amyl alcohol at T > 50 °C as solvent in the absence of water; type C obtained by heating type A to 260 °C ^[14] , type B does not show transition to high temperature form ^[14]																	
T _{dec.} [°C]	Melts before it undergoes violent decomposition ^[14] DSC, T _m = peak T (K): 583.2 @ 1.25 K/min, 583.5 @ 1.25 K/min, 594.4 @ 2.5 K/min, 591.3 @ 2.5 K/min, 594.2 @ 2.5 K/min, 592.7 @ 2.5 K/min, 609.0 @ 10 K/min, 611.0 @ 10 K/min, 608.0 @ 10 K/min, 610.5 @ 10 K/min, 619.0 @ 20 K/min, 620.5 @ 20 K/min, 620.0 @ 20 K/min, 619.5 @ 20 K/min, 633.0 @ 40 K/min, 632.5 @ 40 K/min ^[14]																	
ρ [g cm ⁻³]	1.940 (flotation method @ RT) ^[10] , 1.852 ^[10 as being probably too low] , 1.95 ^[14]																	
Heat of formation	-508.09 ± 3.05 kJ/mol (ΔH _f ^θ) ^[14] , -118.45 kcal/mol (ΔH _f ^θ) ^[14] , 505.8 ± 3.05 kJ/mol (-ΔH _f ^θ , calcd.) ^[14] ,																	
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.															
-Δ _{ex} U° [kJ kg ⁻¹]																		
T _{ex} [K]																		
p _{C-J} [kbar]																		
VoD [m s ⁻¹]																		
V ₀ [L kg ⁻¹]																		
Trauzl test [cm ³ , % TNT]	Only partial explosion, no measureable expansion (small lead block, 6.5 mm bore, 1 g sample, pressed into cartridge shell No. 8 with interior cap) ^[7]																	

Initiation efficiency	Can be ignited to deflagration by a rapidly heated bridgewire ^[8]																																																																															
5 s explosion <i>T</i> [°C] Explosion <i>T</i> [°C]	311–316 ^[14]																																																																															
Burn rate [mm/s]	<p>Linear and mass rates of burning @ 1 atm.: <i>u</i> = 1.50 cm/s, <i>m</i> = 2.74 g cm²s⁻¹^[1]</p> <p>Dependence on the burning rate with the initial temperature, <i>T</i>₀, crystals ground to particle size of ~50 μm, pressed into brass tubes of 8 mm diameter to rel. ρ of 0.9–0.99 g, constant pressure bomb in N₂ atmosphere^[6]:</p> <table><tr><th rowspan="2"><i>p</i>, atm.</th><th colspan="7"><i>u</i> (mm/s) @ <i>T</i>₀, °C</th><th rowspan="2">β, 10³, 1/deg</th></tr><tr><th>20</th><th>40</th><th>60</th><th>80</th><th>100</th><th>120</th><th>150</th></tr><tr><td>0.5</td><td>40</td><td>45</td><td>52</td><td>60</td><td>67</td><td>75</td><td>96</td><td>6.7</td></tr><tr><td>1.0</td><td>52</td><td>58</td><td>64</td><td>70</td><td>76</td><td>82</td><td>98</td><td>4.8</td></tr><tr><td>3.0</td><td>68</td><td>74</td><td>79</td><td>82</td><td>90</td><td>93</td><td>106</td><td>3.4</td></tr><tr><td>6.0</td><td>72</td><td>76</td><td>3</td><td>90</td><td>92</td><td>100</td><td>110</td><td>3.2</td></tr><tr><td>10.0</td><td>64</td><td>68</td><td>74</td><td>80</td><td>87</td><td>94</td><td>100</td><td>3.4</td></tr><tr><td>20.0</td><td>42.5</td><td>47</td><td>52</td><td>56</td><td>62</td><td>67</td><td>76</td><td>4.5</td></tr><tr><td>40.0</td><td>30</td><td>35</td><td>40</td><td>45</td><td>50</td><td>56</td><td>68</td><td>6.3</td></tr></table>	<i>p</i> , atm.	<i>u</i> (mm/s) @ <i>T</i> ₀ , °C							β, 10 ³ , 1/deg	20	40	60	80	100	120	150	0.5	40	45	52	60	67	75	96	6.7	1.0	52	58	64	70	76	82	98	4.8	3.0	68	74	79	82	90	93	106	3.4	6.0	72	76	3	90	92	100	110	3.2	10.0	64	68	74	80	87	94	100	3.4	20.0	42.5	47	52	56	62	67	76	4.5	40.0	30	35	40	45	50	56	68	6.3
<i>p</i> , atm.	<i>u</i> (mm/s) @ <i>T</i> ₀ , °C							β, 10 ³ , 1/deg																																																																								
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Solubility [g/mL]	<p>0.22% in MeOH^[5], 0.029% in MeOH (abs.)^[5], <0.00001% in Et₂O^[5], 1.02% in acetone^[5], 0.4% in H₂O^[5], slightly soluble in cold water (0.5 g/100 g water @ 15 °C)^[14], more soluble in hot water (25 g/100 g @ 100 °C)^[14]</p> <p>Aqueous solubility data from^[14]:</p> <table><tr><th><i>T</i> (°C)</th><th>10³ s/mol dm⁻³</th></tr><tr><td>20</td><td>18.9</td></tr><tr><td>25</td><td>24.1</td></tr><tr><td>25</td><td>23.1</td></tr><tr><td>25</td><td>24.2</td></tr><tr><td>25</td><td>23.3</td></tr><tr><td>25</td><td>26.7</td></tr><tr><td>30</td><td>28.2</td></tr><tr><td>30</td><td>33.2</td></tr></table>	<i>T</i> (°C)	10 ³ s/mol dm ⁻³	20	18.9	25	24.1	25	23.1	25	24.2	25	23.3	25	26.7	30	28.2	30	33.2																																																													
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25	26.7																																																																															
30	28.2																																																																															
30	33.2																																																																															
Hygroscopicity	Crystallizes from water as anhydrous salt ^[14]																																																																															

Enthalpy of soln. [kJ/mol]	<p>In water a = mole ratio of PP to water; b = uncertainties are 95% confidence^[14]:</p> <table><tr><th>m (g)</th><th>n^a</th><th>ΔH^Θ (kJ/mol)</th></tr><tr><td>0.5230</td><td>5,678</td><td>50.84</td></tr><tr><td>0.5142</td><td>5,775</td><td>52.18</td></tr><tr><td>0.5133</td><td>5,784</td><td>50.43</td></tr><tr><td>0.5109</td><td>5,811</td><td>52.08</td></tr><tr><td>0.5035</td><td>5,898</td><td>50.50</td></tr><tr><td>0.4459</td><td>6,657</td><td>50.64</td></tr><tr><td>0.4161</td><td>7,136</td><td>51.26</td></tr><tr><td>0.4118</td><td>7,210</td><td>52.26</td></tr><tr><td>0.3614</td><td>8,212</td><td>50.46</td></tr><tr><td>0.1177</td><td>25250</td><td>50.77</td></tr></table> <p>mean = 51.14 ± 0.55^b</p> <p>42 kJ/mol in water (ΔH^Θ_s)^[14]</p>	m (g)	n ^a	ΔH ^Θ (kJ/mol)	0.5230	5,678	50.84	0.5142	5,775	52.18	0.5133	5,784	50.43	0.5109	5,811	52.08	0.5035	5,898	50.50	0.4459	6,657	50.64	0.4161	7,136	51.26	0.4118	7,210	52.26	0.3614	8,212	50.46	0.1177	25250	50.77
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DDT initiation	<p>Effect of donor-charge composition and loading density on DDT reaction, data from ref^[8]:</p> <table><tr><th colspan="2">Reduced-diameter transition charge</th></tr><tr><th>Transition charge</th><th>Acceptor charge</th></tr><tr><td>PETN S^P_o = 330 m²/kg</td><td>PETN S^P_o = 330 m²/kg</td></tr><tr><td>Density = 1.0 g/cm³</td><td>Density = 1.6 g/cm³</td></tr><tr><td>Diameter = 2.5 mm</td><td></td></tr><tr><td>Length = 6.4 mm</td><td></td></tr></table> <p>Ignition voltage = 2.5 V</p>	Reduced-diameter transition charge		Transition charge	Acceptor charge	PETN S ^P _o = 330 m ² /kg	PETN S ^P _o = 330 m ² /kg	Density = 1.0 g/cm ³	Density = 1.6 g/cm ³	Diameter = 2.5 mm		Length = 6.4 mm																						
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Length = 6.4 mm																																		

	Donor charge			Result
	Explosive	(% by mass)	Density (g/cm ³)	D = detonation ND = ignition but no detonation
	KP	100	1.6	ND
	KP	100	1.2	ND
	KP/PETN	90/10	1.6	ND
	KP/PETN	50/50	1.6	ND
	KP/PETN	25/75	1.6	D
	KP/PETN	10/90	1.6	D
	KP/PETN	90/10	1.6	ND
	KP/PETN	50/50	1.2	D
	KP/PETN	25/75	1.2	D
	KP/PETN	10/90	1.2	D
Activation energy to decomposition [kJ/mol]	214.1 ± 1.5 (DSC, Kissinger method) ^[14] , 223.3 ± 1.5 (DSC, Ozawa method) ^[14]			
Heat capacity [J•mol ⁻¹ •K ⁻¹]	$C_{p,m}^0 = 230.13 @ 298.15 \text{ K (calcd.)}^{[15]}$, 275.67 @ 400.00 K (calcd.) ^[15] , 311.11 @ 500.00 K (calcd.) ^[15] , 338.89 @ 600.00 K (calcd.) ^[15] , 359.27 @ 700.00 K (calcd.) ^[15] , 375.41 @ 800.00 K (calcd.) ^[15]			

	Potassium picrate ^[2]	Potassium picrate ^[4]	Potassium picrate ^[10]	Potassium picrate ^[11]	Potassium picrate ^[12]	Potassium picrate ^[14]
Chemical formula	$C_6H_2KN_3O_7$	$C_6H_2KN_3O_7$	$C_6H_2KN_3O_7$	$C_6H_2KN_3O_7$	$C_6H_2KN_3O_7$	$C_6H_2KN_3O_7$
Molecular weight [g mol ⁻¹]	267.19	267.19	267.19	267.19	267.19	267.19
Crystal system	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic
Space group	<i>lbca</i> (73)	<i>lbca</i> (73)	<i>lbca</i> (73)	<i>lbca</i> (73)	<i>lbca</i> (73)	<i>lbca</i> (73)
<i>a</i> [Å]	13.325	13.333(4)	13.33 ± 0.01	7.135	13.316(3)	13.33
<i>b</i> [Å]	19.090	19.112(4)	19.16 ± 0.02	13.332	19.107(5)	19.09
<i>c</i> [Å]	7.140	7.118(5)	7.154 ± 0.005	19.124	7.138(2)	7.14
α [°]	90	90	90	90	90	90
β [°]	90	90	90	90	90	90
γ [°]	90	90	90	90	90	90
<i>V</i> [Å ³]	1,816.23	1,813.81			1,816	
<i>Z</i>	8	8	8	8	8	8
ρ_{calc} [g cm ⁻³]	1.954	1.957			1.95	
<i>T</i> [K]	295	295			295	
					Slow cooling to RT of a hot aqueous soln.	

3 polymorphs reported (A, B and C): type A obtained when an aqueous/alcohol soln. of PA is neutralized with KOH soln.; type B obtained on using methylated at RT or isopropyl alcohol or amyl alcohol at $T > 50\text{ }^{\circ}\text{C}$ as solvent in the absence of water; type C obtained by heating type A to $260\text{ }^{\circ}\text{C}$ ^[14]; crystallizes from water as anhydrous salt^[14].

Flying plate initiation of acceptor explosives, large diameter charges^[8]:

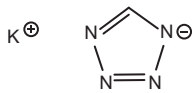
Donor charge			Flying plate			
KP/PETN mixes KP SPO = $250\text{ m}^2/\text{kg}$ PETN SPO = $320\text{ m}^2/\text{kg}$			Flyer material = 6061-T6 Al Flyer barrel: diameter = 2.5 mm Length = 6.4 mm			
Donor charge			Thickness (mm)	Acceptor explosive (density = 1.6 g cm^{-3})	Ignition voltage (V)	Result D = detonation ND = no detonation
KP	PETN	density (g/cm^3)				
(% by mass)						
90	10	1.6	1.27	PETN	40	ND
90	10	1.2	1.27	PETN	40	ND
50	50	1.6	1.27	PETN	40	D
50	50	1.6	1.27	PETN	3	ND
50	50	1.2	1.27	PETN	40	D
50	50	1.6	1.27	9407 PBX	3	ND
25	75	1.6	1.27	PETN	40	D
25	75	1.2	1.27	PETN	40	D
25	75	1.6	1.27	9407 PBX	3	ND
10	90	1.6	1.27	PETN	3	D
10	90	1.6	1.27	PETN	3	D
10	90	1.6	1.27	PETN	40	D
10	90	1.6	1.27	PETN	40	D
10	90	1.6	1.27	PETN	40	D
10	90	1.2	1.27	PETN	3	D
10	90	1.2	1.27	PETN	3	D
10	90	1.6	1.27	9407 PBX	3	D
10	90	1.6	1.27	9407 PBX	40	D
10	90	1.6	1.27	9407 PBX	3	D
10	90	1.6	1.27	9407 PBX	3	ND

10	90	1.6	0.64	9407 PBX	3	D
10	90	1.6	0.64	9407 PBX	3	ND
10	90	1.2	1.27	9407 PBX	3	ND
10	90	1.2	0.64	9407 PBX	3	ND
10	90	1.6	1.27	RDX	40	D

- [1] A. A. Alberts *u.* G. B. Bachman, *J. Am. Soc.* **1935**, 57, 1284.
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- [3] K. Maartmann-Moe, *Acta Cryst.*, **1969**, 25B, 1452–1460.
- [4] G. J. Palenik, *Acta Cryst.*, **1972**, 28B, 1633–1635.
- [5] A. Bolliger, *J. Bio. Chem.*, **1934**, 107, 229–234.
- [6] V. V. Zhalnin, Y. S. Kichin, *Combustion, Explosion Shock Waves*, **1971**, 7, 129–130.
- [7] E. Herz, *Explosive and Process of Making Same*, US Patent 1,443,328A, 23rd January **1923**.
- [8] R. H. Dinegar, *The Ignition and Deflagration of Potassium Picrate (KP) and KP/Explosives Mixtures: Low-Voltage, Nonprimary Detonators*, LA-UR-78-1298, 6th International Pyrotechnics Seminar, Estes Park, Colorado, USA, 17th–21st July **1978**.
- [9] T. E. Larson, P. Dimas, C. E. Hannaford, *Electrostatic Sensitivity Testing of Explosives at Los Alamos*, 9th Int. Symp. on Detonation, Portland, Oregon, USA, vol. II, August 28th–1st September **1989**, pp. 1076–1083.
- [10] M. Bettman, *The Determination of the Crystal Structure of Potassium Picrate*, PhD Thesis, California Institute of Technology, Pasadena, California, USA, **1952**.
- [11] X.-H. Ju, Y.-L. Lu, X.-F. Ma, H.-M. Xiao, *Prop., Expl. Pyrotech.*, **2006**, 31, 290–293.
- [12] J. M. Harrowfield, B. W. Skelton, A. H. White, *Aust. J. Chem.*, **1995**, 48, 1311–1331.
- [13] *LASL Explosive Property Data*, T. R. Gibbs, A. Popolato (eds.), University of California Press, Berkeley, **1980**.
- [14] A. E. Smith, *Thermochemical and Kinetic Aspects of Metal Picrates*, PhD Thesis, University of London, **1983**.
- [15] H.-H. Ju, X.-J. Xu, H.-M. Xiao, *J. Energet. Mater.*, **2005**, 23, 121–130.

Potassium tetrazolate

Name [German, acronym]: Tetrazole, potassium salt [Kaliumtetrazolat]
Main (potential) use: Useful in the synthesis of other energetic compounds
Structural formula:



	Potassium tetrazolate		
Formula	CHN ₄ K		
Molecular mass [g mol ⁻¹]	108.14		
Appearance at RT	Colorless crystals ^[1, 2]		
IS [J]	>100 (BAM) ^[1]		
FS [N]	>360 (BAM) ^[1]		
N [%]	51.81		
Ω(CO ₂) [%]			
T _{m,p.} [°C]	210 (endo, DSC @ 5 °C/min, covered Al pan) ^[1, 2]		
T _{dec.} [°C]	308 (exo, DSC @ 5 °C/min, covered Al pan) ^[1]		
ρ [g cm ⁻³]	1.774 (X-ray @ 200 K) ^[1, 2]		
Heat of formation	174 kJ/mol (ΔH _f ^o , calcd.) ^[1, 2]		
Heat of combustion	−996 kJ/mol ^[1, 2]		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
−Δ _{ex} U ^o [kJ kg ^{−1}]			
T _{ex} [K]			
p _{C-J} [kbar]			
VoD [m s ^{−1}]			
V ₀ [L kg ^{−1}]			
Flame test	Purple-red flame color ^[1, 2]		

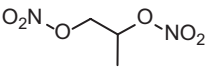
	Potassium tetrazolate ^[1, 2]
Chemical formula	CHKN ₄
Molecular weight [g mol ⁻¹]	108.14
Crystal system	Hexagonal
Space group	<i>P</i> -6 (no. 174)
<i>a</i> [Å]	14.0037(2)
<i>b</i> [Å]	14.0037(2)
<i>c</i> [Å]	10.7285(2)
α [°]	90
β [°]	90
γ [°]	120
<i>V</i> [Å ³]	1,822.03(5)
<i>Z</i>	6
ρ_{calc} [g cm ⁻³]	1.774
<i>T</i> [K]	200
	Colorless crystals from EtOH

[1] J. Stierstorfer, *Advanced Energetic Materials Based on 5-Aminotetrazole – Synthesis, Characterization and Scale-Up*, PhD Thesis, LMU München, Munich, **2009**.

[2] T. M. Klapötke, M. Stein, J. Stierstorfer, *ZAAC*, **2008**, 634, 1711–1723.

Propyleneglycol dinitrate

Name [German, acronym]: Propyleneglycol dinitrate [propylenglykoldinitrat, PGDN]
Main (potential) use: Component of liquid torpedo propellant called Otto fuel^[3]
Structural formula:



	Propyleneglycol dinitrate		
Formula	C ₃ H ₆ N ₂ O ₆		
Molecular mass [g mol ⁻¹]	166.09		
Appearance at RT	Colorless liquid ^[1]		
N [%]	16.87		
Ω(CO ₂) [%]	−28.9		
T _{m,p.} [°C]	−20 ^[3]		
ρ [g cm ⁻³]	1.368 (@ 293 K) ^[1, 2] , 1.37 ^[3]		
Heat of formation			
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
−Δ _{ex} U° [kJ kg ⁻¹]		5.55 MJ/kg (calcd., SD method) ^[4]	
T _{ex} [K]		3,702 (calcd., SD method) ^[4]	
p _{C-J} [kbar]			
VoD [m s ⁻¹]			6,958 (@ 1.37 g cm ⁻³ , D _i) (D _i = ideal detonation velocity) ^[4] 6,573 (@ 1.37 g cm ⁻³ , D _f) (D _f = detonation velocity for critical detonation diameter) ^[4]
V ₀ [L kg ⁻¹]			

Critical diameter [cm]	5.1 mm ^[4]
Trauzl test [cm ³ , % TNT]	155% TNT ^[2] , 540 ^[5] , 540 cm ³ (10 g sample) ^[1]
Vapor pressure [atm. @ °C]	0.0984 Torr @ 25 °C ^[3]
Solubility [g/mL]	Aqueous solubility = 3,500 mg/L @ 25 °C (est.) ^[3] , readily soluble in common organic solvents ^[1] , almost insoluble in water ^[1]
Diffusion coefficient [cm ² /s]	0.077 (air) ^[3] , 7.93×10^{-6} (water) ^[3]
Log K_{ow}	2.66 (est.) ^[3]
Log K_{oc}	2.52 ^[3]
Biodegradation	Undergoes aerobic biodegradation ^[3]

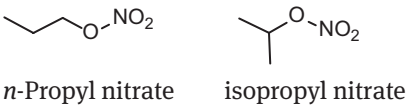
- [1] R. Meyer, J. Köhler, A. Homburg, *Explosives*, 7th edn., Wiley-VCH, Weinheim, **2016**, p. 275.
- [2] B. T. Fedoroff, O. E. Sheffield, *Encyclopedia of Explosives and Related Items*, vol. 2, US Army Research and Development Command, TACOM, Picatinny Arsenal, USA, **1962**.
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Propyl nitrate

Name [German, acronym]: Propyl nitrate, nitric acid propyl ester, (*n*-, *iso*-) propanol nitrate, isopropyl alcohol nitrate [*n*-/iso-propylnitrat, IPN (*iso*-)]

Main (potential) use: *n*-Propyl nitrate: monergol in liquid propellant rockets^[3], *iso*-propyl nitrate: thermobaric explosives^[3], was used as monopropellant prior to hydrazine^[6]

Structural formula:



	Propyl nitrate	
	<i>n</i> -	<i>iso</i> -
Formula	C ₃ H ₇ NO ₃	
Molecular mass [g mol ⁻¹]	105.10	
Appearance at RT	Liquid @ RT (<i>n</i> -) ^[7] , pale yellow liquid with sweet, sickly odor (<i>n</i> -) ^[15] , flammable liquid ^[16]	
IS [J]	>7.4, >49 Nm ^[3] , (H ₅₀ Wg) ⁻¹ = >49 Nm ^[9] , 87 cm (median height, <i>iso</i> -, Rotter apparatus) ^[14]	
FS [N]	>353	
N [%]	13.33	
Ω(CO ₂) [%]	-99.0	
T _{m,p.} [°C]	-122 ^[1]	<0 ^[2]
T _{b,p.} [°C]	110.2 (@ 750 mm Hg) ^[4] , 110.5 ^[7, 8, 16] , bp ₇₆₂ = 110 ^[15]	101.3 (@ 755 mm Hg) ^[4] , 101-102 ^[7, 8, 16] , 102 ^[16]
ρ [g cm ⁻³]	1.058 (@ 293 K) ^[3] , sp. gr. = 1.063 ^[7, 16] , sp. gr. (15°/15°) = 1.0631 ^[7] , sp. gr. (25°/25°) = 1.0531 ^[7] , d ²⁰ ₄ = 1.0538 ^[15]	1.036 (@ 293 K) ^[3] , sp. gr. = 1.054 (@ 0 °C) ^[7] , sp. gr. = 1.036 (@ 19 °C) ^[7] , rel. ρ = 1.036 ^[16]
Heat of formation	-2,041 (enthalpy of form.) ^[3] , -214.6 ± 1.2 kJ/mol (-Δ _f H° @ 298 K, liq.) ^[5] , 174.0 ± 1.3 kJ/mol (Δ _f H° (g)) ^[5]	-2,184 (enthalpy of form.) ^[3] , -229.7 ± 1.2 kJ/mol (-Δ _f H° @ 298 K, liq.) ^[5] , 190.9 ± 1.3 kJ/mol (Δ _f H° (g)) ^[5] , -2,187 kJ/kg (ΔH _i , ICT thermochemical database) ^[10] , -229.3 kJ/mol (enthalpy of form., exptl.) ^[13] , -236.6 kJ/mol (enthalpy of form., calcd., emp.) ^[13]

	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^\circ$ [kJ kg ⁻¹]	4,090	3,126 (calcd., ICT-code, <i>iso</i> -) ^[10] 2,297 (calcd., explosion heat, <i>n</i> -) ^[16]	<i>n</i> -: 3,272 [H ₂ O (l)] ^[3] <i>iso</i> -: 3,126 [H ₂ O (l)] ^[3] 549 kcal/kg [H ₂ O (vapor)] (calcd., <i>n</i> -) ^[7]
T_{ex} [K]	2,598	1,723 (calcd., ICT-code, <i>iso</i> -) ^[10]	
$p_{\text{C-J}}$ [kbar]	95	92.7 MPa (calcd., ICT-code, <i>iso</i> -) ^[10]	
VoD [m s ⁻¹]	5,815 (@ TMD)		7,350
V_0 [L kg ⁻¹]	941		826

High-velocity detonation was not found, it does not propagate in glass tube^[11]. Low-velocity detonation in steel tube (10 mm diameter, 13 mm wall thickness) has been observed^[11].

Trauzl test [cm ³ , % TNT]	15 cm ³ (<i>n</i> -, after correction for expansion produced by detonator) ^[7, 16] , 45 cc (15 cc more than cap alone, 10 g sample, H ₂ O tamping, No. 8 blasting cap, only partial detonation occurred) ^[8]																		
Gap test	<p>scale III (donor = 2 × 20 g pellets of tetryl pressed to $\rho = 1.5$ g mL, each 1.5 in in diameter, Gap = 4 in square cards, charge case = 3 in length of 1½ in steam pipe faced at both ends, hooks, test plate = 3 in square of 16 gage mild steel placed on top of the filled charge case, <i>n</i>-propyl nitrate) critical card value = 16^[12]</p> <p>Probable critical card value^[12]:</p> <table><tr><td>Card value</td><td>Probability</td><td>Card value</td><td>Probability</td></tr><tr><td>13</td><td>0.00001</td><td>16</td><td>0.54</td></tr><tr><td>14</td><td>0.17</td><td>> 16</td><td>0.06</td></tr><tr><td>15</td><td>0.23</td><td></td><td></td></tr></table>			Card value	Probability	Card value	Probability	13	0.00001	16	0.54	14	0.17	> 16	0.06	15	0.23		
Card value	Probability	Card value	Probability																
13	0.00001	16	0.54																
14	0.17	> 16	0.06																
15	0.23																		
Thermal stability	Heating <i>n</i> - isomer may cause it to explode ^[15]																		
Burn rate [mm/s]		<i>iso</i> -: linear burn rate in air atmosphere = 1.42 ± 0.01 mm/s @ 40 bar pressure ^[6] , <i>iso</i> -: burning rate in 14.8% oxygen = 1.39 ± 0.05 mm/s @ 40 bar pressure ^[6]																	

Solubility [g/mL]	Very slightly soluble in water (<i>n</i> -) ^[15] , soluble in EOH, Et ₂ O (<i>n</i> -) ^[15]	
Compatibility	Vapor can form explosive mixture with air with explosion limit 2–100% and flash point = 20 °C, ignition point = 176.7 °C in air ^[16]	
Latent heat of evaporation [kg cal/mol]	7.6 (calcd., <i>n</i> -) ^[4]	7.3 (calcd., <i>iso</i> -) ^[4]
Enthalpy of vaporization, $\Delta_{\text{vis}}H^\circ$ [kJ/mol]	40.6 ± 0.4 (<i>n</i> -) ^[5]	38.8 ± 0.4 (<i>iso</i> -) ^[5]
Refractive index	$n_D^{20} = 1.3979$ (<i>n</i> -) ^[15]	
Dipole moment	2.98 ^[15]	

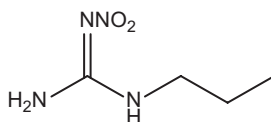
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- [4] G. M. S. Duff, *J. Appl. Chem.*, 5th December **1955**, 642–642.
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Propyl nitroguanidine

Name [German, acronym]: 1-Propyl-2-nitroguanidine, *N*-propyl-*N'*-nitroguanidine [PrNQ]

Main (potential) use: Investigated as a melt-cast binder for insensitive energetic formulations^[1]

Structural formula:



	PrNQ		
Formula	$C_4H_{10}N_4O_2$		
Molecular mass [g mol ⁻¹]	146.15		
Appearance at RT			
IS [J]	DH ₅₀ = >100 (PrNQ, ERL, functionally equivalent to type 12B test; type 12B test = 2.5 kg mass) ^[2] , DH ₅₀ = >100 (PAX-PrNQ, ERL, functionally equivalent to type 12B test; type 12B test = 2.5 kg mass) ^[2]		
FS [N]	>360 (BAM) ^[2] , >360 (PAX-PrNQ, BAM) ^[2]		
ESD [J]	0.25 (no units specified, ABL apparatus operating at 10,000 V) ^[2] , 0.063 (no units specified, ABL apparatus operating at 10,000 V, PAX-PrNQ) ^[2]		
<i>N</i> [%]	38.34		
Ω(CO ₂) [%]	-120.42		
<i>T</i> _{m.p.} [°C]	101.62 (endo onset), 102.48 (endo peak max) (DSC @ 10 °C/min, N ₂) ^[1] , 99–100 ^[3]		
<i>T</i> _{dec.} [°C]	177 (onset of mass loss, TGA @ 10 °C/min, N ₂ , Pt pan) ^[1] , 226.62 (exo onset), 236.26 (exo peak max) (DSC @ 10 °C/min, N ₂) ^[1]		
ρ [g cm ⁻³]			
Heat of formation			
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
-Δ _{ex} <i>U</i> ^o [kJ kg ⁻¹]			
<i>T</i> _{ex} [K]			
<i>p</i> _{C-J} [kbar]			
VoD [m s ⁻¹]			7,760 (@ 1.64 g cm ⁻³ , PAX-PrNQ formulation, rate stick/plate dent method) ^[2]

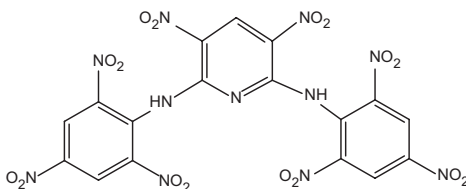
V_0 [L kg ⁻¹]																															
LSGT [cm]	LSGT on PAX-PrNQ, $\rho = 1.65$ g/cc, 50% point = 1.750 in = 175 cards ^[2] : <table border="1"> <thead> <tr> <th>Gap (in)</th><th>Result (go/no go)</th><th>Gap (in)</th><th>Result (go/no go)</th></tr> </thead> <tbody> <tr> <td>1.500</td><td>Go</td><td>1.760</td><td>Go</td></tr> <tr> <td>2.000</td><td>No go</td><td>1.770</td><td>No go</td></tr> <tr> <td>1.750</td><td>Go</td><td>1.770</td><td>No go</td></tr> <tr> <td>1.870</td><td>No go</td><td>1.760</td><td>No go</td></tr> <tr> <td>1.820</td><td>No go</td><td>1.750</td><td>No go</td></tr> <tr> <td>1.780</td><td>No go</td><td>1.750</td><td>No go</td></tr> </tbody> </table>			Gap (in)	Result (go/no go)	Gap (in)	Result (go/no go)	1.500	Go	1.760	Go	2.000	No go	1.770	No go	1.750	Go	1.770	No go	1.870	No go	1.760	No go	1.820	No go	1.750	No go	1.780	No go	1.750	No go
Gap (in)	Result (go/no go)	Gap (in)	Result (go/no go)																												
1.500	Go	1.760	Go																												
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1.750	Go	1.770	No go																												
1.870	No go	1.760	No go																												
1.820	No go	1.750	No go																												
1.780	No go	1.750	No go																												
Thermal stability	177 (onset of mass loss, TGA @ 10 °C/min, N ₂ , Pt pan, mass loss is rapid until ~250 °C then slow to 350 °C at which residual mass loss drops to zero) ^[1]																														
Vapor pressure [Pa]	1.48×10^{-11} Torr @ 25 °C (est.) ^[1] , 9.85×10^{-9} Torr @ 70 °C (est.) ^[1] , 1.52×10^{-6} Torr @ 100 °C (est.) ^[1]																														
Solubility [g/mL]	1.6×10^4 mg/L in H ₂ O (predicted.) ^[1] , soluble in water ^[3] , recryst. from EtOH ^[3]																														
Compatibility	Compatible with RDX, HMX and nitroguanidine ^[1] , stable towards hydrolysis in neutral water ^[1]																														
K_{ow} (log)	1.35 (K_{ow}) ^[1] , 0.13 (log K_{ow}) ^[1]																														
K_{oc} (log)	9.57 (K_{oc}) ^[1] , 0.98 (log K_{oc}) ^[1]																														
ΔH_{dec} [J/g]	796 (DSC @ 10 °C/min, N ₂) ^[1]																														
ΔH_{melt} [J/g]	177 (DSC @ 10 °C/min, N ₂) ^[1]																														
ΔH_{vap} [kJ/mol]	139.7 (est.) ^[1]																														
pH	7 (saturated aqueous soln.) ^[1]																														
Irreversible growth testing	10.63% (average vol. change, 30 temp. cycles between –65°F and 160°F, 3 h at each temperature) ^[2]																														
Exudation testing	0.051 wt.% (cycle –65°F → 160°F, 3 h at each temperature) ^[2]																														

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PYX

Name [German, acronym]: 3,5-Dinitro2,6-bis(picrylmino) pyridine,
2,6-bis(picrylamino)-3,5-dinitropyridine [PYX]
Main (potential) use: Secondary (high) explosive, produced in 300–400 lb/
year quantities for use in thermally stable perforators for
oil and gas wells^[16], replacement for HNS as thermally
stable explosive in commercial applications^[16]

Structural formula:



	PYX									
Formula	C ₁₇ H ₇ N ₁₁ O ₁₆									
Molecular mass [g mol ⁻¹]	621.30									
Appearance at RT										
IS [J]	10 ^[2] , 9 ^[4] , 15.43 ^[5] , 8 ^[6] , 10 ^[6] , 63 cm ^[8] , 9 (ZBL-B instrument) ^[15] , 63 cm (type 12 tool) ^[16, 19] , 84 cm (type 12B tool) ^[16, 19] , 80 cm (AFX-521; 95 wt.% PYX/5 wt.% Kel-F 800, type 12, cf. RDX = 22 cm) ^[19]									
FS [N]	360 ^[1, 6] , 280 (FSKM 10 instrument) ^[15] , negative at all angles ^[16, 19]									
ESD [J]	8.9 ^[1, 5, 20] , 137 mJ ^[1] , 1.00 ^[6] , 0.5 ^[6] , $E_{50\%} = 0.45 \pm 0.06$ (Bruceton formula) ^[13] , $E_{50\%} = 0.49$ (Bruceton formula) ^[13] , $E_{50\%} = 1.18$ (LANL using 0.008 cm Pb foil confinement) ^[13] , 1 (ESD 2008A electric spark tester) ^[15] , 1.175 (0.076 mm foil) ^[16, 19] Data from ^[17] : <table><tr><th colspan="3">50% point energy (J)</th></tr><tr><th>3 mil foil</th><th>10 mil foil</th><th>% expl.</th></tr><tr><td>1.18</td><td>9.00</td><td>0</td></tr></table>	50% point energy (J)			3 mil foil	10 mil foil	% expl.	1.18	9.00	0
50% point energy (J)										
3 mil foil	10 mil foil	% expl.								
1.18	9.00	0								
N [%]	24.80									
Ω(CO ₂) [%]	−55.36									

$T_{m.p.}$ [°C]	460 ^[1, 8, 16] , 360 ^[9, 14] , melts @ 460 °C but begins to rapidly dec. @ 350 °C (DTA @ 20 °C/min) ^[19]		
$T_{dec.}$ [°C]	360 ^[2] , 385 ^[4, 15] , 373 ^[6] , 360 (DSC @ 5 °C/min) ^[6] , 366 (mass loss begins (367 °C onset DSC)), 371 (max. rate of mass loss, exo (374 °C, DSC)) (TG, open pan @ 4 °C/min) – these values shift to lower T if slower heating rates are used ^[11] , 350 (DTA) ^[16, 19] , melts @ 460 °C but begins to rapidly dec. @ 350 °C (DTA @ 20 °C/min) ^[19]		
ρ [g cm ⁻³]	1.88 (crystal, @ 20 °C) ^[1] , 1.77 (gas pycnometry) ^[4] , 1.757 (crystal, @ 298 K) ^[6] , 1.77 (crystal) ^[7] , 1.75 (crystal) ^[8, 16, 19] , 1.77 ^[15] , 1.75 ^[18]		
Heat of formation	43.7 kJ/mol ($\Delta_f H^\circ$) ^[2] , 80.3 ($\Delta_f H$ (heat of form.)) ^[4, 15] , 20.9 kcal/mol ($\Delta_f H^\circ$) ^[7] , 127 kJ/mol ^[1] , 80 kJ/mol ($\Delta_f H$) ^[18]		
Heat of combustion	$\Delta H^\circ_c = -1,858.8$ kcal/mol ^[7]		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{ex}U^\circ$ [kJ kg ⁻¹]	4,780 ^[2]	3,006 (@ 1.75 g cm ⁻³ , calcd. LOTUSES) ^[18]	
T_{ex} [K]	3,609 ^[2]	3,100 (@ 1.75 g cm ⁻³ , calcd. LOTUSES) ^[18]	
p_{CJ} [kbar]	354 ^[3] 251 ^[2]	24.2 GPa (calcd., K-J) ^[4, 15] 25.19 GPa (calcd.) ^[10] 246 ^[7] 25.186 GPa (@ 1.75 g cm ⁻³ , calcd. LOTUSES) ^[18]	242 ^[19]
VoD [m s ⁻¹]	7,757 ^[2] 8,858 ^[3]	7,448 (calcd., K-J) ^[4, 15] 7,500 (@ 1.75 g cm ⁻³ , calcd.) ^[10] 7,480 (@ 1.77 g cm ⁻³) ^[7] 7,497 (@ 1.75 g cm ⁻³ , calcd. LOTUSES) ^[18]	7,450 (no ρ given) ^[19] 7,211 (AFX-521; 95 wt.% PYX/5 wt.% Kel-F 800, rate stick @ 1.70 g cm ⁻³ , pressed ρ) ^[19] 7,202 (AFX-521; 95 wt.% PYX/5 wt.% Kel-F 800, cylinder test @ 1.70 g cm ⁻³ , pressed ρ) ^[19]
V_0 [L kg ⁻¹]	633 ^[2]	989 (@ 1.75 g cm ⁻³ , calcd. LOTUSES) ^[18]	

Critical diameter [cm]	Failure diameter = <2.54 mm ^[16] , failure diameter = <7.62 mm ^[19]
SSGT [cm]	1.02 mm (AFX-521; 95 wt.% PYX/5 wt.% Kel-F 800) ^[19]
Isothermal long-term experiment	RADEX, 100 h @ 260 °C: no dec. or thermal rearrangement occurred ^[6]
Vacuum stability test [cm ³ /days]	@ 200 °C: 0.1/2, 0.1/7, 0.2/14, 0.2/21, 0.2/28, 0.3/35, 0.3/42, 0.4/49, 0.4/56, 0.4/63, 0.5/70, 0.6/77, 0.6/84, 0.7/91 ^[12] 0.5 cm ³ /g/h @ 300 °C ^[16, 19] , 0.9 cm ³ /g/48 h @ 250 °C ^[16, 19] , 0.7 cm ³ /g/91 days @ 200 °C ^[16, 19] 0.02 cm ³ /g/48 h @ 120 °C (AFX-521; 95 wt.% PYX/5 wt.% Kel-F 800) ^[19]
Plate dent test	1.27 cm diameter, confined: 4.01 mm (AFX-521; 95 wt.% PYX/5 wt.% Kel-F 800) ^[19] , 2.54 cm diameter, confined: 7.34 mm (AFX-521; 95 wt.% PYX/5 wt.% Kel-F 800) ^[19] , 2.54 cm diameter unconfined: 4.01 mm (AFX-521; 95 wt.% PYX/5 wt.% Kel-F 800) ^[19]

	PYX^[6]
Chemical formula	C ₁₇ H ₇ N ₁₁ O ₆
Molecular weight [g mol ⁻¹]	621.34
Crystal system	Orthorhombic
Space group	<i>P</i> 2 ₁ 2 ₁ 2 ₁ (no. 19)
<i>a</i> [Å]	14.5179(11)
<i>b</i> [Å]	17.6612(13)
<i>c</i> [Å]	18.3198(14)
α [°]	90
β [°]	90
γ [°]	90
<i>V</i> [Å ³]	4,697.3(6)
<i>Z</i>	8
ρ_{calc} [g cm ⁻³]	1.757
<i>T</i> [K]	298

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Silver azide

Name [German, acronym]: Silver azide, [silberazid, SA]
Main (potential) use: Initiators^[7], small-size detonators
Structural formula:



	Silver azide						
Formula	AgN ₃						
Molecular mass [g mol ⁻¹]	149.9						
Appearance at room temperature (RT)	White crystals ^[14] , white – pale-gray powder (depends on purity), white – gray ^[4, 7] , white crystalline solid, technical product is often gray ^[32] , tends to nucleate a lot so it usually precipitates as a fine powder ^[33] , white (99.9% purity) ^[34] , average size of 105 μ opaque and translucent crystals under microscope (99.9% purity sample) ^[34] , colorless plates and needles (recryst. from aq. ammonia) ^[40]						
IS [J]	<p>1.18 (6 cm, 2 kg mass, 20 mg sample, B.M.)^[4, 5, 7], 1.50 (3 in, 2 kg mass, 18 mg sample, P.A.)^[4, 5, 7], 2–4^[6], 2.5–4 Nm^[8], 3 in (2 kg mass, B.M.)^[11], 6 cm (1 kg mass, B.M.)^[11], 41 cm (500 g mass, B.M.)^[11], <i>H</i>₅₀ = 47.4 cm (ball and disc test)^[14], <i>Fol</i> = 30 (Rotter test)^[14], 77.7 cm (0.5 kg mass, colloidal)^[14], 28.5 cm (0.5 kg mass, coarse crystals)^[14], ~1.2 (B.M.)^[14], ~1.4^[14], 2.0^[14], ~3.8^[14], 777 mm (drop-height of 500 g mass required to cause detonation of colloidal AgN₃)^[21], work = 13.97 kg•m•cm², drop weight = 914 mg, upper limit = 245 cm, lower limit = 150 cm^[22]</p> <p><i>H</i>_{50%}, up–down method, 25 mg samples, pressed to 10 kbar to give pellets of 5 mm diameter, 0.8 mm height; grit was fine, very fine or coarse where stated; PC = polycarbonate^[18]:</p> <table><tr><td>Sample (sample + binder)</td><td>50% height (cm)</td></tr><tr><td>AgN₃ (pure)</td><td>19.3 ± 0.8</td></tr><tr><td>AgN₃ + PC (fine)</td><td>16.8 ± 1.3</td></tr></table> <p>10% point = 11 in (P.A., reduced sensitivity AgN₃ from Costain process, granulation: 18% on 100, 27% on 140, 33% on 200, 18% on 325, 4% through 325)^[29], 50% point = 17 in (P.A., reduced sensitivity AgN₃ from Costain process, granulation: 18% on 100, 27% on 140, 33% on 200, 18% on 325, 4% through 325)^[29], 10% point = 11 in (ball drop, reduced sensitivity</p>	Sample (sample + binder)	50% height (cm)	AgN ₃ (pure)	19.3 ± 0.8	AgN ₃ + PC (fine)	16.8 ± 1.3
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AgN ₃ (pure)	19.3 ± 0.8						
AgN ₃ + PC (fine)	16.8 ± 1.3						

	<p>AgN₃ from Costain process, granulation: 18% on 100, 27% on 140, 33% on 200, 18% on 325, 4% through 325)^[29], 10% point = 7 in (P.A., reduced sensitivity AgN₃ from Costain process, granulation: 17% on 100, 32% on 140, 24% on 200, 22% on 325, 5% through 325)^[29], 50% point = 10 in (P.A., reduced sensitivity AgN₃ from Costain process, granulation: 17% on 100, 32% on 140, 24% on 200, 22% on 325, 5% through 325)^[29], 10% point = 10 in (ball drop, reduced sensitivity AgN₃ from Costain process, granulation: 17% on 100, 32% on 140, 24% on 200, 22% on 325, 5% through 325)^[29], unexplosive point = 4 cm, explosive point = 18 cm (silver sand test, 16.3 g falling mass)^[30], 47.4 cm (ball and disc test)^[31], white and gray (partially decomposed) show equally high sensitivity^[32], particle size has large influence: coarse samples are more sensitive^[32], long needles frequently explode when broken with metal wire^[32], FI = 13–16 (composition RD1336, Rotter apparatus)^[34]</p> <p>Ball and stick apparatus, AgN₃ composition RD1336^[34]:</p> <table><tr><td>Distance of fall (cm)</td><td>12</td><td>14</td><td>16</td><td>19</td><td>21</td></tr><tr><td>% reactions</td><td>4</td><td>18</td><td>38</td><td>76</td><td>88</td></tr></table>	Distance of fall (cm)	12	14	16	19	21	% reactions	4	18	38	76	88																				
Distance of fall (cm)	12	14	16	19	21																												
% reactions	4	18	38	76	88																												
FS [N]	<p>2.6 m s⁻¹ (emergency paper friction test, 50% prob.)^[14], detonates with steel shoe (friction pendulum test)^[7], detonates with fiber shoe (friction pendulum test)^[7], E₅₀ = 5 g^[25], 2.6 m/s (Emery paper test)^[31], white and gray (partially decomposed) show equally high sensitivity^[32]</p> <p>FS (g) tested on porcelain and Emery paper (Julius-Peters BAM)^[20]:</p> <table><tr><th colspan="6">Friction sensitivity (g)</th></tr><tr><th rowspan="2">Porcelain</th><th colspan="5">Emery paper grades</th></tr><tr><th>P80</th><th>P100</th><th>P120</th><th>P180</th><th>P360</th></tr><tr><td>10</td><td>20</td><td>10</td><td>25</td><td>20</td><td>20</td></tr></table> <p>Mallet FS, % ignitions^[35]:</p> <table><tr><th colspan="3">Standard wood mallet on anvils of</th></tr><tr><th>York stone</th><th>Hardwood</th><th>Softwood</th></tr><tr><td>100</td><td>100</td><td>100</td></tr></table> <p>Pendulum FS: failed fiber shoe^[35], failed steel shoe^[35]</p>	Friction sensitivity (g)						Porcelain	Emery paper grades					P80	P100	P120	P180	P360	10	20	10	25	20	20	Standard wood mallet on anvils of			York stone	Hardwood	Softwood	100	100	100
Friction sensitivity (g)																																	
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10	20	10	25	20	20																												
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York stone	Hardwood	Softwood																															
100	100	100																															

	Emery paper FS ^[35] : <table><tr><td>Ignitions/trial at strike velocity (ft/s)</td><td>AgN₃</td></tr><tr><td>3</td><td>0/10</td></tr><tr><td>4</td><td>4/10</td></tr><tr><td>5</td><td>5/10</td></tr><tr><td>7</td><td>5/5</td></tr><tr><td>Type of ignition</td><td>Complete</td></tr></table>	Ignitions/trial at strike velocity (ft/s)	AgN ₃	3	0/10	4	4/10	5	5/10	7	5/5	Type of ignition	Complete									
Ignitions/trial at strike velocity (ft/s)	AgN ₃																					
3	0/10																					
4	4/10																					
5	5/10																					
7	5/5																					
Type of ignition	Complete																					
ESD [J]	<p>0.21 μJ (ignition, advanced test no. 7)^[14], 0.118 μJ (no ignition, advanced test no. 7)^[14], 1.3^[14], 24 mJ (zero ignition probability, uncoated AgN₃)^[25], 18 mJ (zero ignition probability, PVP coated AgN₃)^[25], ignitions @ 0.21 μJ but not @ 0.118 μJ (test no. 7, 42 pF, 100 V and 42 pF, 75 V)^[31], 0.0094–0.017 (Costain)^[33], 0.0094 (Taylor)^[33]</p> <p>Ignition values^[25]:</p> <table><tr><td>Explosive</td><td>Capacitance (MF)</td><td>Voltage (kV)</td><td>Energy (J)</td><td>T (°C)</td><td>RH (%)</td><td>Remarks</td></tr><tr><td>SA (PVP coated)</td><td>0.003</td><td>5.0</td><td>0.0375</td><td>28.5</td><td>40</td><td>Ignited</td></tr><tr><td>SA (uncoated)</td><td>0.001</td><td>8.0</td><td>0.032</td><td>28.3</td><td>41</td><td>Ignited</td></tr></table> <p>0.0094 (P.A., reduced sensitivity AgN₃ from Costain process, granulation: 18% on 100, 27% on 140, 33% on 200, 18% on 325, 4% through 325)^[29], 0.018 (P.A., reduced sensitivity AgN₃ from Costain process, granulation: 17% on 100, 32% on 140, 24% on 200, 22% on 325, 5% through 325)^[29]</p> <p>2.8 × 10⁻⁶ (minimum initiation energy, powder sample, plumb-bob approaching electrode apparatus (contact discharge))^[36], 4 × 10⁻⁴ (conducting rubber electrode (100 Ω resistance) substituted for the base electrode)^[36], 7.5 × 10⁻³ (minimum energy, sieved powder sample passing through 100 mesh but retained on 200 mesh screen, approaching electrode apparatus, 0.50 mm preset gap)^[36], 7 × 10⁻⁴ (minimum energy, subsieve range, approaching electrode apparatus, 0.50 mm preset gap)^[36], crystals of 1.0 × 0.5 × 0.5 mm with electrical resistance of ~10¹² Ω on being subjected to a constant electrical field of 450 V/cm, the current increased through the crystal with time and after several minutes when the current reached 150 μA an explosion occurred^[36]</p>	Explosive	Capacitance (MF)	Voltage (kV)	Energy (J)	T (°C)	RH (%)	Remarks	SA (PVP coated)	0.003	5.0	0.0375	28.5	40	Ignited	SA (uncoated)	0.001	8.0	0.032	28.3	41	Ignited
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N [%]	28.03																					
Ω [%]	0																					

$T_{m.p.}$ [°C]	251 ^[4, 7, 10, 24, 39] , 310 ^[1] , ~250 melts ^[14] , 250 ^[11] , 250 (melts and turns black) ^[14] , 251 (rapid dec. > mpt.) ^[21] , 582 K (DTA @ 5 K/min) ^[23] , 303 (melts followed by dec. in liquid phase, DSC @ 10 °C/min, onset, Al pan with pinhole Al lid) ^[31] , softens @ 250 °C but complete melting does not occur until 300 °C in vacuum (crystalline silver azide) ^[39] , ~250 (dec.) ^[40]		
$T_{\text{phase transition}}$ [°C]	461 ± 2 K (crystallographic transformation, DTA @ 5 K/min) ^[23]		
$T_{\text{dec.}}$ [°C]	>254 (N ₂ evolved) ^[11] , 340 (explosion) ^[13] , 254 (gas liberation) ^[14] , 297–300 (explodes) ^[11] , 303 (@ 10 °C/min, onset) ^[14] , turns slightly violet @ ~150 ^[14] , melts @ 250 and turns black ^[14] , dec. rapidly above mpt. (251 °C) ^[7] , 303 (melts followed by dec. in liquid phase, DSC @ 10 °C/min, onset, Al pan with pinhole Al lid) ^[31] , turns violet @ 150 °C then melts @ 251 °C to black liquid ^[32] , @ 253 °C melt evolves N ₂ gas which gives appearance of boiling ^[32] , 295 (exotherm, onset), ~300 (exotherm peak) Δ°C = 5 (DTA @ 5 °C/min) ^[37]		
ρ [g cm ⁻³]	5.1 (@ 293 K) ^[2, 6] , 5.1 (crystal) ^[7, 14] , 4.8–5.1 ^[11] , 4.81 (crystal) ^[14] , ~1 (bulk ρ , RD1336 AgN ₃ *) ^[14] , 1.6 (bulk ρ , AgN ₃ from Costain process, reduced sensitivity, granulation: 18% on 100, 27% on 140, 33% on 200, 18% on 325, 4% through 325) ^[29] , 1.6 (bulk ρ , AgN ₃ from Costain process, reduced sensitivity, granulation: 17% on 100, 32% on 140, 24% on 200, 22% on 325, 5% through 325) ^[29] , 1.6 (<i>Costain</i>) ^[33] , 1.1 (<i>Taylor</i>) ^[33]		
Heat of formation	213.6 kJ/mol ($\Delta_f H^\circ$) ^[2] , 311 kJ/kg ($\Delta_f H^\circ$) ^[14] , -74.2 kcal/mol (Q_f) ^[11] , 1.86 kJ/g (279.5 kJ/mol) ($\Delta_f H^\circ$) ^[13] , 67.8 kcal/kg ^[7, 16] , 311 kJ/mol ^[14] , 74.17 kcal/mol (standard enthalpy of form. @ 25 °C, cryst.) ^[40]		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{\text{ex}} U^\circ$ [kJ kg ⁻¹]	2,031	65.5 kcal/mol ($Q_{\text{det.}}$) ^[11] 452 kcal/kg ^[16]	452 cal/g ^[7]
T_{ex} [K]	3,471		3,345 ^[11]
p_{C-J} [kbar]	268		90,260 kg/cm ² (@ 3.0 g cm ⁻³ , under 1,100 kg/cm ² press) ^[11]
VoD [m s ⁻¹]	5,372 (@ 4.42 g cm ⁻³ , $\Delta_f H = 312.7$ kJ/mol)	6,800 ^[6] 6,800 (@ 5.1 g cm ⁻³) ^[8]	1,500 (unconfined, hot wire initiation) ^[11, 14] 1,700 (unconfined, initiation by impact with grit particle) ^[11, 14] 1,900 (unconfined, in vacuo @ 0.1 mm Hg pressure) ^[11] 4,000 (@ 4.00 g cm ⁻³) ^[9] 3,830 (@ 2 g cm ⁻³) ^[14]

			4,400 (@ max. obtainable ρ) ^[14] 1,500 (crystals with 0.3–0.4 mm diameter, 1 cm length) ^[14]
V_0 [L kg ⁻¹]	245	244 dm ³ kg ⁻¹ ^[14]	224 ^[10]

Critical diameter [cm]	Needles with 25 μm explode ^[14] , rapid combustion (~7 ms ⁻¹) for diameter ~ 10 μm ^[14]																										
Trauzl test [cm ³ , % TNT]	22.6 cc (for 2 g sample) ^[11] , 115 cm ³ (10 g sample, 38.3% TNT) ^[14] , 88% MF ^[4]																										
Sand test [g]	18.9 g (200 g bomb) ^[4, 7] , 40–43% TNT ^[15] , 41.1 g sand crushed (cf. 37.2 g by MF) ^[11] ,																										
	<table><tr><td>Charge weight SA (g)</td><td colspan="2">Weight of crushed sand (g)</td></tr><tr><td>0.05</td><td colspan="2">1.4</td></tr><tr><td>0.1</td><td colspan="2">3.3</td></tr><tr><td>0.2</td><td colspan="2">6.8</td></tr><tr><td>0.3</td><td colspan="2">10.4</td></tr><tr><td>0.5</td><td colspan="2">18.9</td></tr><tr><td>0.75</td><td colspan="2">30.0</td></tr><tr><td>1</td><td colspan="2">41.1</td></tr></table>			Charge weight SA (g)	Weight of crushed sand (g)		0.05	1.4		0.1	3.3		0.2	6.8		0.3	10.4		0.5	18.9		0.75	30.0		1	41.1	
	Charge weight SA (g)	Weight of crushed sand (g)																									
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	1	41.1																									
Sand crushing power (no. 6 detonator capsule, compressed under 1,000 lb/in ²) ^[21] :																											
<table><tr><td>Weight of charge (g)</td><td>Weight of sand crushed (g)</td><td>Weight of charge (g)</td><td>Weight of sand crushed (g)</td></tr><tr><td>0.05</td><td>1.4</td><td>0.50</td><td>18.9</td></tr><tr><td>0.10</td><td>3.3</td><td>0.75</td><td>30.0</td></tr><tr><td>0.20</td><td>6.8</td><td>1.00</td><td>41.1</td></tr><tr><td>0.30</td><td>10.4</td><td></td><td></td></tr></table>			Weight of charge (g)	Weight of sand crushed (g)	Weight of charge (g)	Weight of sand crushed (g)	0.05	1.4	0.50	18.9	0.10	3.3	0.75	30.0	0.20	6.8	1.00	41.1	0.30	10.4							
Weight of charge (g)	Weight of sand crushed (g)	Weight of charge (g)	Weight of sand crushed (g)																								
0.05	1.4	0.50	18.9																								
0.10	3.3	0.75	30.0																								
0.20	6.8	1.00	41.1																								
0.30	10.4																										

Initiating efficiency	0.02–0.05 g required for complete initiation of TNT ^[7] , 0.05 g for TNT ^[14] , 0.07 g for TNT ^[14]																	
	<table><tr><th>Initiating efficiency (g)^[14]</th><th>Acceptor explosive</th></tr><tr><td>~0.02</td><td>Tetryl</td></tr><tr><td>~0.03</td><td>Picric acid</td></tr><tr><td>~0.07</td><td>Trinitroanisole</td></tr><tr><td>~0.26</td><td>Trinitroxylenes</td></tr><tr><td>~0.25</td><td>TNT</td></tr></table>	Initiating efficiency (g) ^[14]	Acceptor explosive	~0.02	Tetryl	~0.03	Picric acid	~0.07	Trinitroanisole	~0.26	Trinitroxylenes	~0.25	TNT					
	Initiating efficiency (g) ^[14]	Acceptor explosive																
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	~0.07	Trinitroanisole																
	~0.26	Trinitroxylenes																
	~0.25	TNT																
	Influence of processing pressure on min. amount of SA needed to detonate PETN in ¹⁰ / ₁₀ trials (Cu detonator cap, internal diameter = 6.2 mm, no reinforcing cap) ^[14]																	
	<table><tr><td>Pressure on PETN (MPa)^[14]</td><td>0</td><td>196</td><td>196</td><td>196</td><td>196</td></tr><tr><td>Pressure on initiator (MPa)</td><td>0</td><td>0</td><td>49</td><td>98</td><td>147</td></tr><tr><td>Min. initiating charge (g)</td><td>0.005</td><td>0.110</td><td>0.005</td><td>0.005</td><td>0.005</td></tr></table>	Pressure on PETN (MPa) ^[14]	0	196	196	196	196	Pressure on initiator (MPa)	0	0	49	98	147	Min. initiating charge (g)	0.005	0.110	0.005	0.005
Pressure on PETN (MPa) ^[14]	0	196	196	196	196													
Pressure on initiator (MPa)	0	0	49	98	147													
Min. initiating charge (g)	0.005	0.110	0.005	0.005	0.005													
0.05 g is necessary to cause detonation of 0.4 g TNT (no. 6 detonator capsule, whether charge confined by reinforcing cap or not) ^[21]																		
Minimum amount (g) to cause detonation of the secondary explosive ^[21] : 0.02 g for tetryl ^[21] , 0.035 g PA ^[21] , 0.07 g TNT ^[21] , 0.26 g trinitroanisole ^[21] , 0.25 g trinitroxylenes ^[21]																		
Weight of silver azide required for initiation of secondary explosive ^[38] :																		
<table><tr><th colspan="5">Weight (mg)</th></tr><tr><td>RDX</td><td>Tetryl</td><td>Picric acid</td><td>PETN</td><td>TNT</td></tr><tr><td>25</td><td>20</td><td>30</td><td>5</td><td>70</td></tr></table>	Weight (mg)					RDX	Tetryl	Picric acid	PETN	TNT	25	20	30	5	70			
Weight (mg)																		
RDX	Tetryl	Picric acid	PETN	TNT														
25	20	30	5	70														
Dead pressing	AgN ₃ cannot be dead pressed ^[14]																	
5 s explosion <i>T</i> [°C]	297 ^[11, 14] , 297 (microcrystalline powder compressed into pellet of 0.02 g) ^[21] , 290 (5 s, detonates) ^[4, 26] , 337 (297 °C = minimum explosion <i>T</i> , 20 mg sample) ^[37]																	
1 s explosion <i>T</i> [°C] Explosion <i>T</i> [°C]	308 ^[11] , 273 (hot iron dish method) ^[14] 310 (no cap used, 0.1 s) ^[7] , 340 (pure, presence of impurities can lower this to 270 °C) ^[13] , 340 (N ₂ atmosphere @ 26.7 kPa) ^[14] , 273 (spontaneous explosion, varies according to method of heating) ^[21] , 290 (within 20 s, heated Cu capsule in Wood's metal bath) ^[21] , 310 (0.1 s) ^[26] , 300 (on rapid																	

	<p>heating, explodes with high brisance, emits green flash)^[32], 305 (partially decomposed gray sample)^[32], does not explode even at 400 °C under vacuum^[39], 340 (1 s, if nitrogen pressure of 20 cm)^[39], explosion occurs at higher <i>T</i> in thin-walled glass vessels and at lower <i>T</i> when a hot-air furnace is used instead of a liquid bath^[39]</p> <p>Data from^[37]:</p> <table><tr><th>Explosion <i>T</i> (°C)</th><th>Ignition delay (s)</th><th>Sample wt. (mg)</th></tr><tr><td>310–320</td><td>300</td><td>50</td></tr><tr><td>>250</td><td>9</td><td>9</td></tr><tr><td>290</td><td>5</td><td>10</td></tr><tr><td>340</td><td>1</td><td>~ 2</td></tr></table>	Explosion <i>T</i> (°C)	Ignition delay (s)	Sample wt. (mg)	310–320	300	50	>250	9	9	290	5	10	340	1	~ 2	
Explosion <i>T</i> (°C)	Ignition delay (s)	Sample wt. (mg)															
310–320	300	50															
>250	9	9															
290	5	10															
340	1	~ 2															
5 s ignition <i>T</i> [°C] Ignition <i>T</i> [°C]	<p>290 (explodes, USA value)^[7, 16], 310–320 (explodes, Russian value)^[16]</p> <p>273 (dropped onto preheated Wood’s alloy)^[17], 390 (STANNAG)^[14], 300–301^[14], 548 K (deflagration)^[25], 546 K^[28], 351^[30], 352 (instantaneous)^[30], 390 (explodes)^[31]</p>																
Vacuum stability test [cm ³ /h]	<p>0.49/g @ 150 °C for 40 h (reduced sensitivity AgN₃ from Costain process)^[29], 0.34/g @ 150 °C for 40 h (reduced sensitivity AgN₃ from Costain process)^[29], 0.49–0.34/1 g/40 h @ 150 °C (<i>Costain</i>)^[33], 0.40/1 g/40 h @ 150 °C (<i>Taylor</i>)^[33]</p> <p>Data from^[37]:</p> <table><tr><th><i>T</i> (°C)</th><th>Weight (g)</th><th>Time (h)</th><th>Gas evolved (mL, STP)</th></tr><tr><td>150</td><td>1.0</td><td>40</td><td>0.49</td></tr><tr><td>150</td><td>1.0</td><td>40</td><td>0.34</td></tr><tr><td>150</td><td>1.0</td><td>40</td><td>0.40</td></tr></table>	<i>T</i> (°C)	Weight (g)	Time (h)	Gas evolved (mL, STP)	150	1.0	40	0.49	150	1.0	40	0.34	150	1.0	40	0.40
<i>T</i> (°C)	Weight (g)	Time (h)	Gas evolved (mL, STP)														
150	1.0	40	0.49														
150	1.0	40	0.34														
150	1.0	40	0.40														
Volatility	Nonvolatile ^[4] , 0.00 @ 75 °C, 24 h ^[7]																
Thermal stability	No explosion on heating to 400 °C in vacuo ^[14] , heating a single crystal >100 °C causes dec. ^[40]																
Solubility [g/mL]	0.006 g in 100 g H ₂ O @ RT ^[7] , soluble in aqueous NH ₃ @ RT ^[7] , 0.017 g in 100 g Et ₂ O @ RT ^[7] , 0.006 g in 100 g 95% EtOH @ RT ^[7] , 0.015 g in 100 g acetone @ RT ^[7] , practically insoluble in H ₂ O ^[14] , 0.765 mg/100 mL H ₂ O @ 25 °C ^[14] , practically insoluble in common organic solvents ^[14] , soluble in aq. NH ₃ ^[21] , insoluble in nitric acid ^[21] , practically insoluble in water and organic solvents ^[32] , dissolved as a complex by aq. ammonia or anhydrous HF but azide is recovered unchanged after evaporation ^[32] , 8.4 × 10 ^{−3} g/L in water @ 18 °C ^[32] , low solubility in water, values range from 0.001–0.008 g/L ^[33] , 0.006 g/100 g H ₂ O @ 20 °C ^[34] , soluble in aqueous ammonia, KCN ^[34]																

Hygroscopicity	0.04% @ 25 °C in 100% RH ^[7] , nonhygroscopic ^[14] , practically nonhygroscopic ^[4] , nonhygroscopic (reduced sensitivity AgN ₃ from Costain process) ^[29] , nil (<i>Costain and Taylor</i>) ^[33]												
Photosensitivity	Less affected by light than MF or LA ^[7] , 0.19 mJ per mm ² of crystal = critical light absorption for initiation of a crystal ^[14] , light sensitive ^[14] , light sensitive and electron beam ^[23] , turns dark purple when exposed to light ^[30] , photosensitive ^[32] , turns violet then black in light ^[32] , crystals are photoconductors @ RT irradiated with light of correct wavelength, max. photocurrent @ 2,800 Å ^[40] , activation energy for RT photolysis (light λ = 3,650 Å) = ~6 kcal/mol ^[40] , critical light energy for ignition = 39 J (light flash = ~50 μs duration) ^[40]												
Radiation sensitivity	Slow neutron irradiation data from ^[37] :												
	<table><tr><th>Density (g/mL)</th><th>Flux (n/cm²/s)</th><th>Total atoms (per mL)</th><th>Metal nuclei reacting (per second)</th><th>Nitrogen nuclei reacting (per second)</th><th>Nuclear reaction</th></tr><tr><td>0.745</td><td>1 × 10⁸</td><td>1.21 × 10²²</td><td>¹⁰⁷Ag 4 × 10⁶ ¹⁰⁹Ag 1 × 10⁷</td><td>1 × 10⁶</td><td>Silver and nitrogen reactions</td></tr></table>	Density (g/mL)	Flux (n/cm ² /s)	Total atoms (per mL)	Metal nuclei reacting (per second)	Nitrogen nuclei reacting (per second)	Nuclear reaction	0.745	1 × 10 ⁸	1.21 × 10 ²²	¹⁰⁷ Ag 4 × 10 ⁶ ¹⁰⁹ Ag 1 × 10 ⁷	1 × 10 ⁶	Silver and nitrogen reactions
	Density (g/mL)	Flux (n/cm ² /s)	Total atoms (per mL)	Metal nuclei reacting (per second)	Nitrogen nuclei reacting (per second)	Nuclear reaction							
	0.745	1 × 10 ⁸	1.21 × 10 ²²	¹⁰⁷ Ag 4 × 10 ⁶ ¹⁰⁹ Ag 1 × 10 ⁷	1 × 10 ⁶	Silver and nitrogen reactions							
	Minimum ignition energies of white silver azide by light flashes, ^a = small quantity placed in a heated aluminum block and exploded within 30 s ^[37] :												
<table><tr><th>Compound</th><th>Color</th><th>Thermal ignition T (°C)^a</th><th>Electrical energy of flash, half-life 0.8 ms (J)</th><th>Light intensity (J/cm²)</th></tr><tr><td>Silver azide</td><td>White</td><td>250</td><td>310</td><td>2.6</td></tr></table>	Compound	Color	Thermal ignition T (°C) ^a	Electrical energy of flash, half-life 0.8 ms (J)	Light intensity (J/cm ²)	Silver azide	White	250	310	2.6			
Compound	Color	Thermal ignition T (°C) ^a	Electrical energy of flash, half-life 0.8 ms (J)	Light intensity (J/cm ²)									
Silver azide	White	250	310	2.6									
Light-flash ignition energies for silver azide and its mixtures ^[37] :													
	<table><tr><th>Explosive</th><th>Critical flash ignition energy (J)</th></tr><tr><td>Silver azide</td><td>48.0</td></tr><tr><td>Silver azide + 10% PbI₂</td><td>62.0</td></tr><tr><td>Silver azide + 10% HgI₂</td><td>72.0</td></tr></table>	Explosive	Critical flash ignition energy (J)	Silver azide	48.0	Silver azide + 10% PbI ₂	62.0	Silver azide + 10% HgI ₂	72.0				
Explosive	Critical flash ignition energy (J)												
Silver azide	48.0												
Silver azide + 10% PbI ₂	62.0												
Silver azide + 10% HgI ₂	72.0												
	Initiated by irradiation with electron pulses of nanosecond duration ^[13]												
Compatibility	Dec. in nitric acid ^[7, 32] , unaffected by water and CO ₂ ^[7] , dec. as suspension in boiling water ^[32]												
Dielectric breakdown	Time to breakdown = <1 s in d.c. field of ≥400 kV m ⁻¹ ^[19] , 5 days @ 15 kV m ⁻¹ ^[19]												

$\Delta H_{\text{melting}}$ [kJ kg ⁻¹]	104 ± 2 (DTA @ 5 K/min) ^[23]					
Enthalpy of soln. [kcal/mol]	16.67 ^[40]					
Specific heat [kJ kg ⁻¹ K ⁻¹]	0.29 ± 0.04 (465–530 K temperature range, DTA @ 5 K/min) ^[23] , 0.117 cal/g/°C @ 250 °C ^[40]					
Explosive power	192,000 kg m, 1.097% MF ^[7]					
Hardness [kg mm ⁻²]	51.9 ± 2.6 (single crystals, @ 20 °C, Vicker's hardness) ^[24]					
Frictional properties	Frictional properties @ 20 °C with sliding velocity of 0.20 mms ⁻¹ ^[24] :					
	μ (coefficient of friction at high loads)	τ_0 (constant)	α (constant)	μ_{cal} (calcd. coefficient of friction at high loads)	μ (coefficient of friction for single crystal on single crystal)	-(l-m)
	0.40	1.01×10^7 Pa	0.42 ± 0.01	0.44 ± 0.02		0.37
Firing times of hot bridgewire initiators	Firing times of hot bridgewire initiators, 50 mg sample loads, voltage of 450 V ^[26] :					
	Milling time, h	Capacitance, μF				
		0.05	0.05	0.0047		
	24	1.13–1.47	1.17–1.56	1.9–3.1		
	64	1.23–1.89	1.23–2.36	1.3–43.1		
Laser sensitivity	SA can be successfully initiated using a UV excimer laser ^[2] :					
	Pressing force, KN	Detonator type	Nominal wavelength, nm	Energy density, KJ/m ²	Function time (μs)	Source
	1 KN	Confined	249	0.4	0.5	Excimer laser
	10 KN	Confined	249	0.4	1.5	Excimer laser
Sensitiveness	13.97 N cm ² (work) ^[28]					

M59 detonator transition charge test	Data from ^[29] :					
	Transition material	Charge weight (mg)	RDX weight (mg)	Test holder	Witness material	indent depth (in)
	AgN ₃	60	68	Brass	Aluminum	0.0599
	AgN ₃	110	34	Brass	Aluminum	0.0520
	AgN ₃	60	68	Brass	aluminum	0.0630
Dielectric constant, <i>k</i>	9.35 (log-frequency, frequency = 1.35 mc/s) ^[40]					
Miscellaneous	Applying an electric field to crystals will cause detonation at <i>T</i> as low as −100 °C ^[13]					

	RT-AgN ₃ ^[1]	HT-AgN ₃ ^[3]	HP-AgN ₃ ^[12]	AgN ₃ ^[40]
Chemical formula	AgN ₃	AgN ₃	AgN ₃	AgN ₃
Molecular weight [g mol ^{−1}]	149.9	149.9	149.9	149.9
Crystal system	Orthorhombic	Monoclinic	Tetragonal	Orthorhombic
Space group	<i>I b a m</i> (no. 72)	<i>P 2₁/ c</i> (no. 14)	<i>I 4/ m c m</i> (no. 140)	
<i>a</i> [Å]	5.600(1)	6.0756(2)	5.52(2)	5.59
<i>b</i> [Å]	5.980(6)	6.1663(2)	5.52(2)	5.91
<i>c</i> [Å]	5.998(1)	6.5729(2)	5.57(1)	6.01
α [°]	90	90	90	90
β [°]	90	114.2(1)	90	90
γ [°]	90	90	90	90
<i>V</i> [Å ³]	200.86	224.62(1)	169.722	
<i>Z</i>	4	4		4
ρ_{calc} [g cm ^{−3}]	4.957	4.4324		
<i>T</i> [K]	298	442		
			@ 2.7 GPa pressure	

* RD1336 AgN₃ is produced by adding aqueous HNO₃ to an almost neutral solution of NaN₃/AgNO₃/aq. NH₃

Long colorless crystals of AgN₃ which explode on breaking are obtained from aqueous ammonia^[7].

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Silver fulminate

Name [German, acronym]: Silver fulminate, silver oxidoazaniumylidynemethane^[9]
[silberfulminat, knallsilber]

Main (potential) use: Historically as primary explosive, very small amounts used in firework torpedoes, snaps and crackers^[9], unsuitable for military applications, for example, as stab-sensitive material due to its extreme sensitivity^[11], detonators used by the Italian Navy^[11], small quantities in pyrotechnics, fireworks, snaps, pull-crackers and paper caps^[11]

Structural formula:



	Silver fulminate
Formula	AgCNO
Molecular mass [g mol ⁻¹]	149.9
Appearance at RT	White crystals with silky luster ^[8] , colorless crystals/white powder ^[9] , white crystalline material ^[11] , fine needles (crude product) ^[11]
IS [J]	~0.8–1.9 ^[4] , unexplosive point = ≤1 cm, explosive point = 8 cm (silver sand test, falling mass = 8.6 g) ^[8] , Fol = 22 (Rotter test, cf. RDX Fol = 80, commercial silver fulminate) ^[11] Ball and disc: 15 cm = ⁶ / ₁₀ fires ^[11] , 13 cm = ⁶ / ₁₀ fires ^[11] , 12 cm = ⁴ / ₁₀ fires ^[11] , 11 cm = ⁴ / ₁₀ fires ^[11] , 10 cm = ³ / ₁₀ fires ^[11] , 9 cm = ¹ / ₁₀ fires ^[11] , 8 cm = ⁰ / ₂₀ fires (commercial silver fulminate) ^[11]
FS [N]	Emery paper: 2.5 ft/s (~0.76 m/s) = ⁷ / ₁₀ fires ^[11] , 2.0 ft/s (~0.6 m/s) = ⁵ / ₁₀ fires ^[11] , 1.5 ft/s (~0.45 m/s) = ⁰ / ₁₀ fires (commercial silver fulminate) ^[11]
ESD [J]	Metal/metal electrodes 0.04 μJ @ 48 pF (commercial silver fulminate) ^[11] , rubber/metal electrodes 0.3 μJ @ 48 pF (commercial silver fulminate) ^[11]
N [%]	9.34
Ω(CO ₂) [%]	
T _{phase transition} [°C]	Two polymorphic forms detected using X-ray diffraction (orthorhombic and trigonal (rhombohedral)) but no amorphous form detected ^[11] , no phase changes between 20 and 145 °C (DTA) ^[11]
T _{dec.} [°C]	Explodes @ 186–193 °C (@ 0.2 °C/min) ^[4] , 170 (explodes in 5 s) ^[5]
ρ [g cm ⁻³]	3.938 (@ 293 K) ^[1] , 4.107 (orthorhombic crystals) ^[4] , 3.796 (trigonal crystals) ^[4]
Heat of formation	179 kJ/mol (Δ _f H°) ^[4] , 361.5 kJ/mol (ΔH _f °, dimer), 1.21 kJ/g ^[10] , 180 kJ/mol (enthalpy of form.) ^[9]

	Calcd. (EXPLO5 6.03)	Exptl.
$-\Delta_{\text{ex}}U^{\circ}$ [kJ kg ⁻¹]		1,970 kJ mol ⁻¹ (calorimeter) ^[4]
T_{ex} [K]		
$p_{\text{C-J}}$ [kbar]		
VoD [m s ⁻¹]		~1,700 (average VoD, for ~0.5 mm thick unconfined film ignited by hot wire, no ρ specified) ^[11]
V_0 [L kg ⁻¹]		

Sand test [g]	Essentially the same brisance as that of mercury fulminate (MF) ^[11]
Initiation efficiency	Minimum amount (g) which causes detonation in secondary explosive ^[7] : 0.02 g for tetryl ^[7] , 0.05 g for PA ^[7] , 0.095 g for TNT ^[7] , 0.23 g for trinitroanisole ^[7] , 0.30 g for trinitroxyethylene ^[7] , ~15 times more efficient as MF for exploding tetryl, but only about 30% more efficient for exploding TNX ^[11]
5 s explosion T [°C] Ignition T [°C]	170 ^[5, 7] 245 (dropped onto preheated Wood's alloy) ^[6] , 225 (instantaneous) ^[8] , 200 (exploded, commercial silver fulminate) ^[11] , 204 (exploded, commercial silver fulminate) ^[11] , 170 ^[11]
Thermal stability	Sample stored under water for 40 years darkened in color but showed no change in other physical or chemical properties ^[11]
Solubility [g/mL]	0.75 g dissolved in 1 L H ₂ O @ 13 °C ^[7] , 0.18 g dissolved in 1 L H ₂ O @ 30 °C ^[7] , slightly soluble in water: 0.075 g/100 mL H ₂ O @ 13 °C ^[11] , 0.25 g/100 mL H ₂ O @ 100 °C ^[11] , insoluble in nitric acid ^[11]
Hygroscopicity	Nonhygroscopic ^[11]
Photosensitivity	Darkens on exposure to light ^[7, 11] , not very sensitive to light ^[8]
Compatibility	Violent explosion on contact with H ₂ S ^[10] , dec. in hydrochloric acid ^[11]
Radiation sensitivity	Crystals warped under exposure to X-rays during data collection ^[11] , ignition on exposure to intense light from Xe-filled flash bulb ^[11]
Stab sensitivity	Relatively stab insensitive – 1.7 g stab igniters containing 10 mg silver fulminate failed to function with input energies ≤ 25 in ounces (~176 mJ), only positive response achieved with 60 mg pressed in one increment @ 10 in ounces ^[11]
Dead pressed	@ loads >33 MPa ^[11]

	Silver fulminate ^[1, 3]	Silver fulminate ^[2, 3]
Chemical formula	AgCNO	AgCNO
Molecular weight [g mol ⁻¹]	149.89	149.89
Crystal system	Trigonal	Orthorhombic

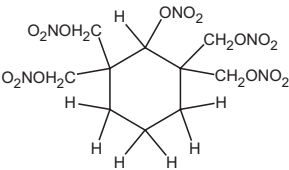
Space group	<i>R</i> -3	<i>C m c m</i> (no. 63)
<i>a</i> [Å]	9.109 ± 0.015	3.864 ± 0.006
<i>b</i> [Å]		10.722 ± 0.018
<i>c</i> [Å]		5.851 ± 0.010
α [°]	115.44	90
β [°]		90
γ [°]		90
<i>V</i> [Å ³]	393.3	242.4
<i>Z</i>	6	4
ρ_{calc} [g cm ⁻³]	3.796	4.107
<i>T</i> [K]	297	

Crystals grown from 6M ammonia formed as needles and leaflet clusters. Both polymorphs appeared as both types of crystals (needles and leaflets) and could not be distinguished under the microscope^[11].

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Sixolite

Name [German, acronym]: Tetramethylolcyclohexanol pentanitrate, nitrohexanol
Main (potential) use: under research
Structural formula:



	Sixolite			
Formula	C ₁₀ H ₁₅ N ₅ O ₁₅			
Molecular mass [g mol ⁻¹]	445.25			
Appearance at RT	Pale yellow solid ^[2]			
IS [J]				
FS [N]				
ESD [J]				
N [%]	15.73			
Ω(CO ₂) [%]	-44.9			
T _{m,p.} [°C]	122.5 ^[2]			
T _{dec.} [°C]				
ρ [g cm ⁻³]	1.44 ^[2]			
Heat of formation	170.39 kcal/mol (-ΔH _f , heat of form. @ standard conditions) ^[3] , -357 kcal/kg (enthalpy of form.) ^[4]			
Heat of combustion	exptl. heat of combustion data ^[3] :			
	-ΔU _{B/M} (cal/g)	-ΔU _B (kcal/mol)	-ΔU _R (kcal/mol @ 1 atm. and constant vol.)	-ΔH _R (kcal/mol @ 1 atm. and constant pressure)
	2,900.94 ± 2.41	1,291.67	1,290.42	1,286.72
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.	
-Δ _{ex} U ^o [kJ kg ⁻¹]		3,765.6 ^[2]		
T _{ex} [K]				

p_{CJ} [kbar]			
VoD [m s ⁻¹]		7,430 (@ 1.58 g cm ⁻³) ^[5]	
V_0 [L kg ⁻¹]			

Trauzl test [% TNT]	135 ^[5]
Ballistic mortar test [% TNT]	127 ^[5]

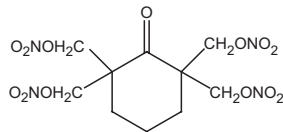
- [1] J. P. Agrawal, R. D. Hodgson, *Organic Chemistry of Explosives*, John Wiley and Sons Ltd., **2007**, pp. 73–74.
- [2] J. Liu, *Nitrate Esters Chemistry and Technology*, Springer, **2019**.
- [3] G. Stegeman, *Heat of Combustion of Explosive Substances*, OSRD No. 5306, Division 8 National Defense Research Committee of the Office of Scientific Research and Development, USA, 4th July **1945**.
- [4] S. M. Kaye, *Encyclopedia of Explosives and Related Items*, vol. 9, US Army Research and Development Command, TACOM, Picatinny Arsenal, USA, **1980**.
- [5] B. T. Fedoroff, O. E. Sheffield, *Encyclopedia of Explosives and Related Items*, vol. 2, US Army Research and Development Command, TACOM, Picatinny Arsenal, USA, **1962**.

Sixonite

Name [German, acronym]: Tetramethylolcyclohexanone tetranitrate, 2-oxo-1,1,3,3-tetrakis-nitryloxymethyl-cyclohexane, 1,1,3,3-tetrakis-nitryloxymethyl-cyclohexanone-(2), 2,2,6,6-tetrakis (nitryloxymethyl) cyclohexanone, cyclohexanone tetranitrate

Main (potential) use: flashless propellant

Structural formula:



	Sixonite																	
Formula	C ₁₀ H ₁₄ N ₄ O ₁₃																	
Molecular mass [g mol ⁻¹]	398.24																	
Appearance at RT																		
IS [J]	<div>Design no. 3 apparatus^[4]:</div> <table><tr><th>Drop height (cm)</th><th>Trials</th><th>% explosions</th></tr><tr><td>80</td><td>20</td><td>40</td></tr><tr><td>85</td><td>20</td><td>40</td></tr><tr><td>90</td><td>20</td><td>55</td></tr><tr><td>95</td><td>20</td><td>55</td></tr></table> <div>$H_{50} > 90$ cm (design no. 3 apparatus)^[4], $H_{50} = 29$ cm (design no. 5 apparatus)^[4], H_{50} (av.) = 120 cm (design no. 9, 2.5 kg hammer)^[4], $H_{50} = 46$ cm (2.5 kg hammer, design no. 11)^[4], $H_{50} = 47.5$ cm (design no. 12, 63 units cf. TNT = 100 units)^[4]</div>			Drop height (cm)	Trials	% explosions	80	20	40	85	20	40	90	20	55	95	20	55
Drop height (cm)	Trials	% explosions																
80	20	40																
85	20	40																
90	20	55																
95	20	55																
FS [N]																		
ESD [J]																		
N [%]	14.07																	
Ω(CO ₂) [%]	−56.2																	
T _{m.p.} [°C]	55–56 ^[1, 6] , 66 ^[2]																	
T _{dec.} [°C]																		
ρ [g cm ^{−3}]																		

Heat of formation	182.24 kcal/mol ($-\Delta H_f$, heat of form. @ standard conditions) ^[3]		
Heat of combustion	Exptl. heat of combustion data ^[3] :		
	$-\Delta U_{B/M}$ (cal/g)	$-\Delta U_B$ (kcal/mol)	$-\Delta U_R$ (kcal/mol @ 1 atm. and constant vol.)
	$-\Delta H_R$ (kcal/mol @ 1 atm. and constant pressure)		
	3,127.70 ± 1.33	1,245.59	1,243.67
	1,240.71		
	$Q_c^V = 3,153 \text{ cal/g}^{[6]}$		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^o$ [kJ kg ⁻¹]		3,451.8 ^[2]	
T_{ex} [K]			
p_{C-J} [kbar]			
VoD [m s ⁻¹]		7,740 (@ 1.51 g cm ⁻³) ^[2, 5]	25,400 ft/s (@ 1.4 g cm ⁻³) ^[1]
V_0 [L kg ⁻¹]			

Ballistic mortar test [% TNT]	114 ^[5, 6]
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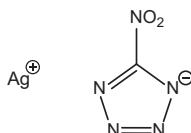
- [1] Department of the Army Technical Manual, *EOD Information for Solid and Liquid Propellants, Conventional Explosives, and Other Dangerous Materials*, TM 9-1385-211, Headquarters, Department of the Army, USA, January **1969**.
- [2] J. Liu, *Nitrate Esters Chemistry and Technology*, Springer, **2019**.
- [3] G. Stegeman, *Heat of Combustion of Explosive Substances*, OSRD No. 5306, Division 8 National Defense Research Committee of the Office of Scientific Research and Development, USA, 4th July **1945**.
- [4] H. D. Mallory, *The Development of Impact Sensitivity Tests at the Explosives Research Laboratory Bruceton, Pennsylvania During the Years 1941–1945*, NAVORD Report 4236, US Naval Ordnance Laboratory, White Oak, Maryland, USA, 16th March **1956**.
- [5] B. T. Fedoroff, O. E. Sheffield, *Encyclopedia of Explosives and Related Items*, vol. 2, US Army Research and Development Command, TACOM, Picatinny Arsenal, USA, **1962**.
- [6] S. M. Kaye, *Encyclopedia of Explosives and Related Items*, vol. 9, US Army Research and Development Command, TACOM, Picatinny Arsenal, USA, **1980**.

Silver nitrotetrazolate

Name [German, acronym]: 5-Nitro-(1*H*)-tetrazole silver salt [Silber nitrotetrazolat]

Main (potential) use: Investigated as possible component of detonant/stab sensitive composition, possible future lead-free initiator (detonant class)^[3], possible use as initiating primers^[4]

Structural formula:



	Silver nitrotetrazolate		
Formula	CN ₅ O ₂ Ag		
Molecular mass [g mol ⁻¹]	221.91		
Appearance at RT	Creamy-tan colored, free flowing solid ^[3] , white, felt-like needles ^[4]		
IS [J]	Ball and disc (A polymorph): 4 cm, 6/10 fires ^[1] ; 2½ cm, 4/50 fires ^[1] ; 2 cm, 2/50 fires ^[1] , <1 ^[2] , 22.7 cm (ball and disc test) ^[3]		
FS [N]	Emery friction (A polymorph): 4 ft/s, 5/5 fires ^[1] ; 3 ft/s, 2/20 fires ^[1] ; 2 ft/s, 1/20 fires ^[1] ; 1½ ft/s, 0/20 fires ^[1] , <5 ^[2] , 1.7 m/s (Emery paper test) ^[3]		
ESD [J]	Minimum electrostatic energy to fire metal/metal electrodes = 12 µJ (A polymorph) ^[1] , <50 mJ ^[2] , ignitions @ 45 µJ (standard test) ^[3] , ignition @ 2.6 µJ but not @ 1.9 µJ (test no. 7) ^[3]		
N [%]	31.56		
Ω(CO ₂) [%]			
T _{m,p.} [°C]	Explodes @ 262 °C ^[3]		
T _{dec.} [°C]	254 (onset, DSC @ 10 °C/min, Al pan with Al pinhole lid) ^[3]		
Heat of formation			
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
-Δ _{ex} U° [kJ kg ⁻¹]			
T _{ex} [K]			
p _{C-J} [kbar]			
VoD [m s ⁻¹]			
V ₀ [L kg ⁻¹]			

Initiating efficiency	Exceeds that of LA for tetryl ^[4] , 0.005 g against tetryl ^[4]
5 s explosion T [°C] Ignition T [°C] Explosion T [°C]	265 (@ 5 °C/min, A polymorph) ^[1] , 259 (explodes) ^[3] 340 ^[3] , ~230 (detonates) ^[4]
Vacuum stability test [cm ³ /h]	0.3% mass loss @ 100 °C, 0.2 mm Hg vacuum for 1 week (A polymorph) ^[1] , 4.5% mass loss @ 230 °C, 1 mm pressure, 1 h (A polymorph) ^[1]
Solubility [g/mL]	Difficultly soluble in water ^[4]
Hygroscopicity	Inflammability not influenced by moisture
Compatibility	Not unduly susceptible to hydrolysis ^[1] , less susceptible to attack by vapors from plastic or rubber than LA or silver azide ^[1] , reacts rapidly with tetrazene at high humidity and high T ^[1] , incompatible with Al under humid conditions ^[1] , more corrosive towards Al than to Cu ^[1] , does not affect stainless steel ^[1] , stable in nitric acid solution ^[4] , inflammability not influenced by moisture ^[4] ,
Stab sensitivity	Insensitive ^[1]
ERDET test [wt. found to detonate RDX in an ERDET]	30 mg (A polymorph) ^[1]
Dead pressing	Dead pressed @ 46 MN/m ² (A polymorph) ^[1] , prone to dead pressing ^[3]

Six types of silver nitrotetrazolate were found using X-ray powder photography patterns, however, only three were isolated pure: A, D and F^[1]

A = main product from nitric acid solns.^[1]; A = main product from neutral solns. in admixture with D and E^[1]; F = main product from ammonia solns.^[1]; D = obtained pure from simultaneous addition of sodium nitrotetrazolate and AgNO₃ to dil. aq. ammonia followed by neutralization with dil. nitric acid^[1]

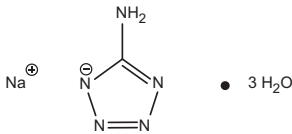
- [1] J. M. Jenkins, J. R. White, *The Salts of 5-Substituted Tetrazoles: Part 3: Further Investigations into the Preparation and Properties of Silver 5-Nitrotetrazole and Mercuric 5-Nitrotetrazole*, Technical Report No. 172, Explosives Research and Development Establishment, Waltham Abbey, Essex, UK, February **1974**.
- [2] T. M. Klapötke, J. Stierstorfer, *Energetic Tetrazole N-Oxides*, Ch. 6 in *Green Energetic Materials*, T. Brinck (ed.), Wiley, **2014**.
- [3] R. W. Millar, *Lead-Free Initiator Materials for Small Electro-Explosive Devices for Medium Caliber Munitions: Final Report 04 June 2003*, QinetiQ Ltd., Farnborough, U.K., May **2003**.
- [4] E. von Herz, *C-Nitrotetrazole Compounds*, US Patent 2,066,954, January 5th **1937**.

Sodium 5-aminotetrazolate trihydrate

Name [German, acronym]: Sodium aminotetrazolate trihydrate [natrium 5-aminotetrazolat trihydrat]

Main (potential) use: In the synthesis of other tetrazole-based energetic materials^[1]

Structural formula:



	Sodium 5-aminotetrazolate trihydrate		
Formula	CH ₈ N ₅ NaO ₃		
Molecular mass [g mol ⁻¹]	161.11		
Appearance at RT	Colorless crystals ^[1]		
IS [J]			
FS [N]			
ESD [J]			
N [%]	43.47		
Ω(CO ₂) [%]			
T _{m.p.} [°C]	306 (DSC @ 5 °C/min, covered Al pans) ^[1]		
T _{dec.} [°C]	Loses water @ T < 100 °C in several steps (DSC @ 5 °C/min, covered Al pan) ^[1]		
ρ [g cm ⁻³]	1.54 (X-ray) ^[1]		
Heat of formation	−1,136 kJ/mol (Δ _f H°) ^[1]		
Heat of combustion	Δ _c H = −657 kJ/mol (exptl.) ^[1] , Δ _c U = −980 cal/g (@ C ^v , bomb calorimetry) ^[1]		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
−Δ _{ex} U° [kJ kg ⁻¹]			
T _{ex} [K]			
p _{C-J} [kbar]			
VoD [m s ⁻¹]			
V ₀ [L kg ⁻¹]			
I _s [s]			
Thermal stability	Loses H ₂ O on standing in air ^[1]		
Hygroscopicity	Loses water on standing in air ^[1]		
Flame test	Orange flame color ^[1]		

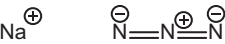
	Sodium 5-aminotetrazole trihydrate ^[1]
Chemical formula	$\text{NaCH}_8\text{N}_5\text{O}_3$
Molecular weight [g mol^{-1}]	161.11
Crystal system	Triclinic
Space group	$P\bar{1}$ (no. 2)
a [Å]	5.8689(7)
b [Å]	10.0258(9)
c [Å]	12.171(1)
α [°]	87.34(1)
β [°]	77.546(9)
γ [°]	80.059(9)
V [Å ³]	688.76(13)
Z	4
ρ_{calc} [g cm^{-3}]	1.554
T [K]	200

- [1] J. Stierstorfer, *Advanced Energetic Materials Based on 5-Aminotetrazole – Synthesis, Characterization and Scale-Up*, PhD Thesis, LMU München, Munich **2009**.

Sodium azide

Name [German, Acronym]: Sodium azide, sodium trinitride^[11], Smite^[11]
[Natriumazid]
Main (potential) use: Gas generator for safety systems, for example,
airbags^[11], reagent in energetic materials synthesis^[11],
preparation of lead azide^[12, 21], automotive airbags and
other nitrogen gas generators^[13]

Structural formula:



	Sodium azide
Formula	NaN ₃
Molecular mass [g mol ⁻¹]	65.01
Appearance at RT	Colorless crystals/white powder ^{r[11]} , white crystalline solid ^[13] , white salt ^[14] , white, odorless crystalline solid ^[21, 22]
IS [J]	Not sensitive ^[14] , 15 m], $P_c = 0.8 \pm 0.05$ GPa @ $H_0 = 0.7$ mm (10 kg mass, K-44-2 vertical impact testing machine, testing device no. 2) ^[18]
FS [N]	not sensitive ^[14]
ESD [J]	
N [%]	64.64
Ω(CO ₂) [%]	
T _{m,p.} [°C]	275 (dec.) ^[11, 21, 22]
T _{b,p.} [°C]	300 @ 1.013 hPa (vigorous dec.) ^[22]
T _{phase transition} [°C]	β - → α - (compression @ 294 K) ^[1] , α - → γ - (compression under 2.8 GPa @ 333 K) ^[1] , γ - → α - (decompression @ ambient T) ^[1] , NaN ₃ adopts two different phases at atmospheric pressure depending on the T: rhombohedral ($R\bar{3}m$, high T, β -form, $T > 292$ K) ^[1] and monoclinic ($C2/m$, low T, α -form) ^[1] , β - → α - (T_c (transition T) between 285–296 K) ^[1] , no phase transitions on heating β - to its $T_{dec.}$ @ 548 K ^[1] , unit cell of a monoclinic form @ ~1.0 GPa (diamond-anvil cell technology) consistent with LT α -form ^[1] , β - → α - occurs @ 0.07 GPa and the formed α -form remains stable to the highest pressures studied ^[1] , three pressure induced phase transitions observed (diamond anvil cell): 0.3 GPa (α - → β -), 17.3 GPa and 28.7 GPa ^[1] , β - → γ - (compression of β -form @ ~257 K between 2.6 and 3.0 GPa) ^[1] , 0.25 GPa (α - → β -) ^[1] , α - does not undergo phase transition @ 290 K @ pressures up to 6.06 GPa ^[1] , above 287 K (phase I) NaN ₃ = $R3m$ ($Z = 1$), below 287 K (phase II) NaN ₃ = $C2/m$ ($Z = 1$) ^[16] , 292.2 K (HT rhombohedral phase → LT monoclinic phase) ^[17] , lower T form = α -NaN ₃ , higher T form = β -NaN ₃ ^[19] , 13 (α - → β -, value probably too low) ^[19] , ~18

	(single crystal changes appearance probably due to cleavage, flaking which is sharp, reversible and reproducible) ^[19] , 291–294 K transition T ^[20]																												
	<p>548 K (@ atmospheric pressure)^[1], 275^[13], 365 (heating in nitrogen)^[14], 275 (melts with dec.)^[21]</p> <p>DTA (Alumina open crucible, 20 °C/min, air, powdered NaN₃): 400 (small exotherm), 450 (onset, large exotherm), 460 ± 9 (exo, peak max.), mass loss @ 450 = ~60%^[2], DTA (Alumina open crucible, 20 °C/min, NaN₃ tablet, air): 402 ± 2 (larger exotherm cf. powder sample)^[2], DTA (Alumina open crucible, 20 °C/min, N₂ atmosphere): 440 (exotherm corresponding to ~5% mass loss (average value from 10 mins.))^[2], DTA (Alumina open crucible, 20 °C/min, Ar atmosphere): 440 (exotherm)^[2], DTA (Alumina open crucible, 20 °C/min, He atmosphere): 460 (exotherm)^[2]</p> <p>DTA (Alumina open crucible, 20 °C/min, Ar atmosphere) on milled samples (particle size = 4.8 µm after 6 h milling, 2.5 µm after 48 h milling)^[2]:</p> <table><tr><th>Milling time (h)</th><th>DTA exotherm peak max. (°C)</th><th>Milling time (h)</th><th>DTA exotherm peak max. (°C)</th></tr><tr><td>0</td><td>~ 450</td><td>~ 24</td><td>~ 400</td></tr><tr><td>5</td><td>~ 450</td><td>~ 50</td><td>~ 390</td></tr><tr><td>~12</td><td>~ 420</td><td></td><td></td></tr></table> <p>DTA (Alumina open crucible, 20 °C/min, air) on milled samples^[2]:</p> <table><tr><th>Particle size (µm)</th><th>DTA exotherm peak max. (°C)</th><th>Particle size (µm)</th><th>DTA exotherm peak max. (°C)</th></tr><tr><td>>105</td><td>~ 463</td><td>44–77</td><td>~ 480</td></tr><tr><td>74–105</td><td>~ 470</td><td>< 44</td><td>~ 485</td></tr></table> <p>Aging in N₂: purity = 460 °C after 0 h storage^[2], 460 °C after 8 h storage^[2], ~457 °C after 12 h storage^[2], ~458 °C after 24 h storage^[2], ~458 °C after 48 h storage^[2]</p> <p>Aging in Ar: 460 °C (8 h storage)^[2], ~455 °C (18 h storage)^[2]</p> <p>Aging in CO₂ saturated by H₂O: ~455 °C (24 h storage)^[2], ~447 °C (48 h storage)^[2]</p> <p>Aging in dried CO₂: ~458 °C (8 h storage)^[2], ~454 °C (12 h storage)^[2], ~453 °C (24 h storage)^[2], ~452 °C (49 h storage)^[2]</p> <p>Aging in O₂: ~457 °C (8 h storage)^[2], ~453 °C (12 h storage)^[2], ~454 °C (24 h storage)^[2], ~454 °C (48 h storage)^[2]</p>	Milling time (h)	DTA exotherm peak max. (°C)	Milling time (h)	DTA exotherm peak max. (°C)	0	~ 450	~ 24	~ 400	5	~ 450	~ 50	~ 390	~12	~ 420			Particle size (µm)	DTA exotherm peak max. (°C)	Particle size (µm)	DTA exotherm peak max. (°C)	>105	~ 463	44–77	~ 480	74–105	~ 470	< 44	~ 485
Milling time (h)	DTA exotherm peak max. (°C)	Milling time (h)	DTA exotherm peak max. (°C)																										
0	~ 450	~ 24	~ 400																										
5	~ 450	~ 50	~ 390																										
~12	~ 420																												
Particle size (µm)	DTA exotherm peak max. (°C)	Particle size (µm)	DTA exotherm peak max. (°C)																										
>105	~ 463	44–77	~ 480																										
74–105	~ 470	< 44	~ 485																										
ρ [g cm ⁻³]	1.85 ^[11] , 1.846 ^[12] , sp. gr. = 1.846 ^[13] , 1.850 (rel. ρ) ^[13] , 1.846 @ 20 °C ^[21] , 1.85 @ 20 °C ^[22]																												
Heat of formation	5.09 kcal/mol (ΔH°_f , exptl.) ^[3] , 6.12 kcal/mol (ΔH°_f , calcd.) ^[3] , 5.08 kcal/mol (standard enthalpy of formation, cryst., @ 25 °C) ^[24] , 21.7 kJ/mol (enthalpy of form.) ^[11]																												

	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^{\circ}$ [kJ kg ⁻¹]			
T_{ex} [K]			
$p_{\text{C-J}}$ [kbar]			
VoD [m s ⁻¹]			Does not propagate even when LA is exploded near it ^[23]
V_0 [L kg ⁻¹]			
Thermal stability	<p>NaN₃ exposed in a dessicator @ RT to flowing gas environments^[2]: Aging in N₂ (no aging observed after 48 h): purity = ~98.5% after 0 h storage^[2], purity = ~98.5% after 12 h storage^[2], purity = ~98.5% after 24 h storage^[2], purity = ~98.5% after 48 h storage^[2] Aging in O₂: purity = ~98.5% after 0 h storage^[2], purity = ~97% after 12 h storage^[2], purity = ~95% after 24 h storage^[2], purity = ~94% after 48 h storage^[2] Aging in CO₂ (g) saturated by H₂O: purity = ~98.5% after 0 h storage^[2], purity = ~94% after 8 h storage^[2], purity = ~92% after 18 h storage^[2], purity = ~90% after 24 h storage^[2], purity = ~48% after 48 h storage^[2] Aging in dried CO₂: purity = ~98.5% after 0 h storage^[2], purity = ~97% after 8 h storage^[2], purity = ~96% after 12 h storage^[2], purity = ~95% after 24 h storage^[2], purity = ~91% after 48 h storage^[2] Dec. on heating into sodium and nitrogen^[12], stable for several years in sealed containers @ RT^[21]</p>		
Vapor pressure [atm. @ °C]	1 Pa @ 20 °C ^[21] , 0.01hPa @ 20 °C ^[22]		
Burn rate [mm/s]	1.2 ± 0.1 psi @ 1,000 psi, rel. vol. gas per vol. generant = 0.97 (NaN ₃ baseline) ^[10] , 1.3 ± 0.2 psi @ 1,000 psi, rel. vol. gas per vol. generant = 1.0 (NaN ₃ low sulfur) ^[10]		
Solubility [g/mL]	41 g/100 g H ₂ O @ 20 °C ^[11] , 40.16% in H ₂ O @ 10 °C ^[12] , 41.7% in H ₂ O @ 17 °C ^[12] , 0.3% in EtOH @ 25 °C ^[12] , insoluble in Et ₂ O ^[12] , soluble in liq. NH ₃ ^[12] , 30–42% @ 20 °C in water ^[13] , dissolves readily in water: 28% w/w @ 0 °C, 29.5% w/w @ 21 °C, 34% w/w @ 80 °C, 35.5% w/w @ 100 °C ^[14] , less readily soluble in 1,2-ethanediol, 2-methoxyethanol, formamide ^[14] , practically insoluble in EtOH, Et ₂ O, acetone, THF, toluene, CHCl ₃ , 2-butanone, methyl acetate methyl urethane ^[14] , 40.8 g dissolve in 100 mL H ₂ O @ 20 °C ^[18] , 41.0 g/100 g H ₂ O @ 15 °C ^[21] , 420 g/L H ₂ O @ 17 °C ^[22]		
Compatibility	Incompatible with acids, heavy metals and materials which contain heavy metals (e.g., brass) ^[13] , contact with water may form HN ₃ ^[13] , incompatible with liquids and vapors of low pH ^[13] , incompatible with CS ₂ , halogenated hydrocarbons ^[13]		

Dielectric constants	Dielectric constants and losses versus crystal orientation ^[4] :			
	Orientation	k'	k''	ω
	$\langle 111 \rangle$	$17 \pm 2.0 \times 10^{-2}$	$10^3 - 10^6$	
pH	9.0 ^[13]			
$\log P_{ow}$	0.3 (<i>n</i> -octanol/water) ^[22]			
Thermal conductivity	25×10^{-4} c.g.s. units (mean $T = 68$ °C, pellet density = 1.77 g/cc) ^[24]			
Enthalpy of soln. [kcal/mol]	3.17 (@ 25 °C) ^[24]			

	Sodium azide α -NaN ₃ ^[9]	NaN ₃ ^[5, 6, 9]	NaN ₃ ^[7]	NaN ₃ ^[8]	γ -NaN ₃ ^[1] (NaN ₃ -III)	α -NaN ₃ ^[1]
Chemical formula	NaN ₃	NaN ₃	NaN ₃	NaN ₃	NaN ₃	NaN ₃
Molecular weight [g mol ⁻¹]	65.01	65.01	65.01	65.01	65.01	65.01
Crystal system	Monoclinic	Trigonal	Trigonal	Trigonal	Tetragonal	Monoclinic
Space group	$C2/m$ (no. 12)	$R\bar{3}m$ (166)	$R3m$ (160)	$R\bar{3}m$ (166)	$I4/mcm$	$C2/m$ (no. 12)
a [Å]	6.211	5.481	5.499	3.646	5.6114(3)	5.9019(6)
b [Å]	3.658	5.481	5.499	2.646		3.5414(3)
c [Å]	5.323	5.481	5.499	15.223	6.0418(4)	5.0732(9)
α [°]	90	38.72	38.72	90		90
β [°]	108.43	38.72	38.72	90		104.45(1)
γ [°]	90	38.72	38.72	120		90
V [Å ³]	114.735	57.9	58.480	175.252	190.24(2)	103.12(2)
Z		1	1	3		
ρ_{calc} [g cm ⁻³]	1.88175	1.85				
T [K]						
					Powder diffraction @ 3.30 GPa, 393 K	Powder diffraction @ 3.22 GPa, 393 K

	$\text{NaN}_3^{[15]}$	$\alpha\text{-NaN}_3^{[19]}$	$\beta\text{-NaN}_3^{[19]}$	$\beta\text{-NaN}_3^{[20]}$	$\text{NaN}_3^{[24]}$
Chemical formula	NaN_3	NaN_3	NaN_3	NaN_3	NaN_3
Molecular weight [g mol^{-1}]	65.01	65.01	65.01	65.01	65.01
Crystal system	Monoclinic	Monoclinic	Rhombohedral	Rhombohedral	Body-centered rhombohedral
Space group	$C2/m$ (no. 12)	$C2/m$ (no. 12)	$R\bar{3}m$ (166)	$R\bar{3}m$ (166)	
a [Å]	6.1654(5)	6.211	3.646 ± 0.002	Used unit cell parameters from ^[19]	
b [Å]	3.6350(3)	3.658			5.488
c [Å]	5.2634(6)	5.323	15.213 ± 0.005		
α [°]	90	90			
β [°]	107.543(5)	108.43			
γ [°]	90	90			
V [Å ³]					
Z		2	1		1
ρ_{calc} [g cm^{-3}]					
T [K]	12			300	
		Powder X-ray diffraction @ 90 – –100 °C; powder ground but not sieved	Single crystal data, RT	Powder neutron diffraction	

$\alpha\text{-NaN}_3$ = monoclinic ($C2m$)^[9], $\beta\text{-NaN}_3$ = rhombohedral ($R\bar{3}m$)^[9], crystallizes as β -form from 1,2-ethanediol, 2-methoxyethanol and formamide^[14]

variation in the cell parameters of $\alpha\text{-NaN}_3$ with pressure^[1]:

P (GPa)	a (Å)	b (Å)	c (Å)	β (°)	V (Å ³)
0.00	6.3027(4)	3.6526(2)	5.4525(8)	111.551(9)	116.75(1)
0.09	6.2785(4)	3.6552(2)	5.4070(7)	110.458(8)	116.26(1)
0.19	6.2483(4)	3.6529(2)	5.3654(7)	109.490(8)	115.45(1)
0.37	6.2169(3)	3.6478(2)	5.3284(6)	108.687(7)	114.47(1)
0.79	6.1476(4)	3.6305(2)	5.2588(6)	107.212(9)	112.11(1)

1.29	6.0720(4)	3.6069(2)	5.1935(6)	105.860(7)	109.41(1)
1.54	6.0228(4)	3.5901(2)	5.1570(5)	105.086(7)	107.66(1)
2.17	5.9664(4)	3.5689(2)	5.1160(5)	104.237(7)	105.59(1)
2.87	5.9122(4)	3.5474(2)	5.0802(5)	103.494(7)	103.61(1)
3.29	5.8687(4)	3.5298(2)	5.0536(6)	102.909(7)	102.04(1)
3.84	5.8259(4)	3.5111(2)	5.0280(6)	102.376(8)	100.46(1)
4.42	5.7879(5)	3.4931(2)	5.0061(6)	101.931(8)	99.03(1)
5.02	5.7510(5)	3.4766(2)	4.9859(7)	101.506(9)	97.68(1)
5.66	5.7175(6)	3.4606(2)	4.9685(7)	101.128(10)	96.46(1)
6.06	5.6924(12)	3.4474(5)	4.9552(14)	100.836(20)	95.51(3)

Unit cell parameters for NaN_3 from variable temperature and pressure neutron powder diffraction; pattern @ 300 K/2.47 GPa is a mixed phase of both α - and γ - forms^[1]:

T (K)	P (GPa)	Form	a (Å)	b (Å)	c (Å)	β (°)	V (Å ³)
294	0.13	β -	3.64684(17)		15.222(3)		175.32(3)
294	0.70	α -	6.1721(11)	3.6373(6)	5.2817(19)	107.66(3)	113.00(4)
294	1.23	α -	6.0907(12)	3.6139(6)	5.2061(18)	106.11(2)	110.10(4)
294	1.91	α -	6.0055(10)	3.5826(5)	5.1422(14)	104.82(2)	106.96(3)
333	2.19	α -	5.9838(11)	3.5749(5)	5.1316(15)	104.57(2)	106.24(3)
333	2.46	α -	5.9224(10)	3.5493(5)	5.0836(14)	103.64(2)	103.85(3)
338	3.03	α -	5.9139(9)	3.5476(5)	5.0841(14)	103.59(2)	103.68(3)
350	3.03	α -	5.9118(5)	3.5459(2)	5.0802(7)	103.55(1)	103.53(1)
373	3.14	α -	5.9091(5)	3.5439(2)	5.0802(7)	103.53(1)	103.41(1)
393	3.20	α -	5.9073(7)	3.5430(3)	5.0802(10)	103.53(1)	103.37(2)
393	3.22	α -	5.9019(6)	3.5414(3)	5.0732(9)	104.45(1)	103.12(2)
393	3.30	γ -	5.6114(3)		6.0418(4)		190.24(2)
393	3.33	γ -	5.5965(3)		6.0136(4)		188.35(2)
383	3.47	γ -	5.5962(4)		6.0092(6)		188.20(3)
373	3.34	γ -	5.5957(4)		6.0093(5)		188.17(3)
363	3.35	γ -	5.5950(3)		6.0096(4)		188.13(2)
353	3.24	γ -	5.5947(4)		6.0076(5)		188.04(2)
343	3.29	γ -	5.5943(3)		6.0063(5)		187.97(2)
333	3.28	γ -	5.5937(3)		6.0047(4)		187.88(2)

313	3.27	γ -	5.5932(3)		6.0023(4)		187.78(2)
300	2.47	γ - α -	5.6169(4) 5.933(3)	3.5512(2)	6.0553(6) 5.079(5)	103.96(7)	191.04(3) 103.85(9)
300	1.32	α -	6.068(2)	3.6006(9)	5.187(3)	105.85(4)	109.02(6)
300	0.00	α -	6.2957(14)	3.6573(8)	5.434(2)	110.70(3)	117.04(5)

Cell constants of NaN_3 from single crystal data^[15]:

T (K)	a (Å)	b (Å)	c (Å)	β (°)
160	6.2233(42)	3.6510(27)	5.3359(25)	108.444(37)
210	6.2467(40)	3.6573(25)	5.3642(25)	109.092(40)
228	6.2614(58)	3.6579(39)	5.3842(25)	109.522(55)
253	6.2764(31)	3.6558(25)	5.4178(16)	110.108(23)
272	6.3043(40)	3.6613(35)	5.4285(27)	110.802(37)
280	6.3016(43)	3.6566(43)	5.4265(29)	111.106(35)
282	6.3105(40)	3.6578(20)	5.4830(20)	111.212(30)
295	6.3264(48)	3.6525(28)	5.4902(41)	112.593(43)

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Sodium chlorate

Name [German, acronym]: Sodium chlorate [natrium chlorat]
Main (potential) use: Pyrotechnics, component of initiating high explosives and propellant compositions
Structural formula:



	Sodium chlorate	
Formula	NaClO ₃	
Molecular mass [g mol ⁻¹]	106.40	
Appearance at RT	White powder, colorless odorless crystals or white granules ^[8]	
N [%]	0	
Ω(CO ₂) [%]		
T _{m,p.} [°C]	248 ^[1, 8] , 248–261 ^[6]	
T _{dec.} [°C]	356 ^[2] , ~300 (liberates oxygen) ^[8]	
ρ [g cm ⁻³]	2.50 ^[1] , 2.488 ^[3] , 2.490 (@ 15 °C) ^[6] , 2.5 ^[8]	
Heat of formation	–805 cal/g ^[3]	
	Calcd. (EXPLO5 6.03)	Exptl.
–Δ _{ex} U° [kJ kg ⁻¹]		
T _{ex} [K]		
p _{C-J} [kbar]		
VoD [m s ⁻¹]		
V ₀ [L kg ⁻¹]		

Solubility [g/mL]	82 parts per 100 parts H ₂ O @ 0 °C ^[7] , 204 parts per 100 parts H ₂ O @ 100 °C ^[7]
Hygroscopicity	Hygroscopic ^[7]
Compatibility	Should not be in contact with organic substances or other oxidizable substances ^[8]
pH	Aqueous soln. is neutral ^[8]

	NaClO₃ ^[4]	NaClO₃ ^[5]
	Ambient pressure, RT, phase-I [†]	Metastable, high temperature phase-III
Chemical formula	NaClO ₃	NaClO ₃
Molecular weight [g mol ⁻¹]	106.40	106.40
Crystal system	Cubic	Monoclinic
Space group	<i>P</i> 2 ₁ 3 (no. 198)	<i>P</i> 2 ₁ / <i>a</i>
<i>a</i> [Å]	6.570(6)	8.78(5)
<i>b</i> [Å]	6.570(6)	5.17(5)
<i>c</i> [Å]	6.570(6)	6.88(5)
α [°]	90	90
β [°]	90	110
γ [°]	90	90
<i>V</i> [Å ³]	283.59	293.47
<i>Z</i>		
ρ_{calc} [g cm ⁻³]		
<i>T</i> [K]		

[†] common form = cubic crystals^[6]

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Sodium nitrate

Name [German, acronym]: Sodium nitrate, soda niter^[12, 13], nitratine^[12], sodium saltpeter^[12], sodium salt of nitric acid^[12], cubic nitre^[12, 13], nitrate of soda^[12], Chile niter^[12], Chile saltpeter^[12, 13] [natronsalpeter, natriumnitrat, SN]

Main (potential) use: In industrial explosives, oxidizer in blasting powder^[5]

Structural formula:



	SN	
Formula	NaNO ₃	
Molecular mass [g mol ⁻¹]	85.0	
Appearance at RT	Crystalline, white solid ^[8] , colorless, transparent crystals, white granules or powder ^[13]	
N [%]	16.48	
Ω(CO ₂) [%]		
T _{phase transitions} [°C]	206–273 (endo), DTA transition T= 273 (rhombic → trigonal) ^[6]	
T _{m,p.} [°C]	310 ^[1, 12] , 317 ^[5] , 306.8 ^[8] , 308 (onset, endo), 311 (endo, peak max, DSC @ 20 °C/min) ^[10] , 308 ^[13]	
T _{dec.} [°C]	380 (DSC @ 5 °C/min) ^[11] , 380 ^[8] , ~605 (start of dec. TGA @ 10 °C/min, 5–10 mg sample, covered Al pans) ^[9] , DTA (@ 15 °C/min): 304 (fusion), 628 (slight bubbling), 642 (rapid bubbling), 710 (slight nitrous fumes), 777 (vigorous nitrous fumes) ^[6] , no exotherm peak <450 °C (DSC @ 20 °C/min) ^[10]	
ρ [g cm ⁻³]	2.260 (@ 293 K) ^[2] , 2.259 ^[4] , 2.265 ^[5] , 2.261 ^[8] . 2.26 ^[12, 13]	
Heat of formation	–423 kJ/mol (Δ _f H°) ^[3] , –5,503 kJ/kg (Δ _f H°) ^[3] , –1,312 kJ/kg ^[4] , –445.9 kJ/mol (H _f) ^[8] , –468 kJ/mol (enthalpy of form.) ^[12]	
	Calcd. (EXPLO5 6.03)	Exptl.
–Δ _{ex} U° [kJ kg ⁻¹]		
T _{ex} [K]		
p _{C-J} [kbar]		
VoD [m s ⁻¹]		
V ₀ [L kg ⁻¹]		

C_p [J/mol K]	103.2 ^[8]
Solubility [g/mL]	Highly H ₂ O soluble ^[8] , 15.8 g soluble in 100 g <i>N,N</i> -DMF @ 60 °C ^[8] , 91 g/100 g H ₂ O @ 25 °C ^[12] , 1 g in 1.1 mL H ₂ O ^[13] , 1 g in 0.6 mL boiling water ^[13] , 1 g in 125 mL EtOH ^[13] , 1 g in 52 mL boiling EtOH ^[13] , 1 g in 3,470 mL abs. alcohol ^[13] , 1 g in 300 mL abs. MeOH, dissolving in water lowers the temperature ^[13]
Hygroscopicity	Very hygroscopic ^[8] , usually used as prills due to its strong H ₂ O affinity ^[8] , critical humidity = 77.5% RH @ 20 °C ^[11] , deliquescent in moist air ^[13]
Heat of melting [J/g]	31 (DSC @ 20 °C/min) ^[10]
pH	Aqueous soln. is neutral ^[13]

	NaNO ₃ ^[7]	NaNO ₃ ^[7]	NaNO ₃ ^[7]
Chemical formula	NaNO ₃	NaNO ₃	NaNO ₃
Molecular weight [g mol ⁻¹]	85.0	85.0	85.0
Crystal system	Trigonal	Trigonal	Trigonal
Space group	$R\bar{3}c$ (no. 167)	$R\bar{3}c$ (no. 167)	$R\bar{3}m$ (no. 166)
a [Å]	5.0655(5)	5.0660(5)	5.0889(5)
b [Å]	5.0655(5)	5.0660(5)	5.0889(5)
c [Å]	16.577(3)	16.593(3)	8.868(3)
α [°]			
β [°]			
γ [°]			
V [Å ³]	368.4	368.8	204.6
Z	6	6	3
ρ_{calc} [g cm ⁻³]			
T [K]	100	120	563
	Synchrotron	Neutron diffraction	Neutron diffraction

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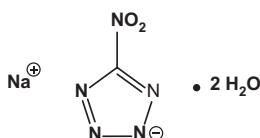
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Sodium 5-nitrotetrazolate dihydrate

Name [German, acronym]: Sodium nitrotetrazolate dihydrate, [natrium nitrotetrazolat dihydrat, NaNT]

Main (potential) use: Precursor for synthesis of DBX-1^[1], useful precursor for the synthesis of Pb-free primary explosives^[2]

Structural formula:



	NaNT•2H ₂ O		
Formula	CH ₄ N ₅ NaO ₄		
Molecular mass [g mol ⁻¹]	173.06		
Appearance at RT	Colorless – light-yellow crystals ^[1] , off-white solid or crystals ^[2]		
IS [J]	>30 (BAM) ^[2]		
FS [N]	~360 (BAM) ^[2]		
N [%]	40.47		
Ω(CO ₂) [%]			
T _{m,p.} [°C]	75 (H ₂ O loss, DSC @ 5 °C/min) ^[2] , highly exothermic dec. without melting ^[2]		
T _{dec.} [°C]	200 (DSC @ 5 °C/min) ^[2] , highly exothermic dec. without melting ^[2]		
ρ [g cm ⁻³]	1.731 (X-ray) ^[2]		
Heat of formation	360 kJ/mol (Δ _f H°) ^[2]		
Heat of combustion	Δ _c U = 1,200(20) cal/g (exptl., @ constant volume) ^[2] , Δ _c H = 850(20) kJ/mol (exptl.) ^[2]		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
–Δ _{ex} U° [kJ kg ⁻¹]			
T _{ex} [K]			
p _{C-J} [kbar]			
VoD [m s ⁻¹]			
V ₀ [L kg ⁻¹]			
Solubility [g/mL]	Recryst. from acetone ^[1, 2] , soluble in acetone ^[2]		
Flame sensitivity	Explodes ^[2]		

	NaNT•2H₂O ^[2]
Chemical formula	CH ₄ N ₅ NaO ₄
Molecular weight [g mol ⁻¹]	173.08
Crystal system	Triclinic
Space group	<i>P</i> -1
<i>a</i> [Å]	6.4266(9)
<i>b</i> [Å]	7.875(2)
<i>c</i> [Å]	8.180(3)
α [°]	104.66(2)
β [°]	109.78(2)
γ [°]	110.28(2)
<i>V</i> [Å ³]	331.7(2)
<i>Z</i>	2
ρ_{calc} [g cm ⁻³]	1.731
<i>T</i> [K]	200

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Sodium perchlorate

Name [German, acronym]: Sodium perchlorate [natriumperchlorat]
Main (potential) use: Manufacture of other perchlorates, used in flares, incendiaries
Structural formula:



*Sodium perchlorate is often obtained as a hydrate^[5]

	Sodium perchlorate	
Formula	NaClO ₄	
Molecular mass [g mol ⁻¹]	122.4	
Appearance at RT	Colorless crystals ^[5] , white powder, white deliquescent crystals (monohydrate) ^[12]	
IS [J]	<i>H</i> _{50%} >320 cm ^[8]	
<i>N</i> [%]	0	
Ω(CO ₂) [%]	+52.3 (Na ₂ O + HCl)	
<i>T</i> _{phase transitions} [°C]	313 (rhombohedral → cubic) ^[8] , 175–313 (endotherm), DTA transition <i>T</i> = 313 (rhombic → cubic, DTA @ 15 °C/min) ^[3]	
<i>T</i> _{m.p.} [°C]	473 (crystals) ^[8]	
<i>T</i> _{dec.} [°C]	482 (DSC @ 5 °C/min) ^[1, 5] , 480 ^[8] , 473 (fusion), 527 (slight bubbling), 578 (vigorous bubbling) (DTA @ 15 °C/min) ^[3]	
ρ [g cm ⁻³]	2.52 ^[1] , 2.54 ^[5] , 2.5298 ^[8] , 2.536 (@ 25 °C) ^[8]	
Heat of formation	−305.9 kJ/mol (Δ _f <i>H</i> ^o) ^[2] , −3,130 kJ/kg (enthalpy of form.) ^[5] , −750 cal/g ^[4] , −91.48 kcal/mol (<i>Q</i> _f) ^[8] , −91.56 kcal/mol (Δ <i>H</i> ^o _f , exptl.) ^[9] , −93.46 kcal/mol (Δ <i>H</i> ^o _f , calcd.) ^[9]	
	Calcd. (EXPLO5 6.03)	Exptl.
−Δ _{ex} <i>U</i> ^o [kJ kg ⁻¹]		
<i>T</i> _{ex} [K]		
<i>p</i> _{C-J} [kbar]		
VoD [m s ⁻¹]		
<i>V</i> ₀ [L kg ⁻¹]		

Solubility [g/mL]	51.4 g/100 g MeOH ^[11] , 14.7 g/100 g EtOH ^[11] , 4.0 g/100 g <i>n</i> -propanol ^[11] , 1.0 g/100 g <i>n</i> -butanol ^[11] , 51.7 g/100 g acetone ^[11] , insoluble in Et ₂ O ^[11] , very soluble in water ^[12] , readily soluble in water and EtOH ^[5]
Hygroscopicity	Hygroscopic ^[5] , deliquescent crystals (monohydrate) ^[12]
$\Delta H^\circ_{\text{sol}}$ [kcal/mol]	$3.32 \pm 0.08^{[10]}$, $3.347 \pm 0.005^{[10]}$

	NaClO ₄ ^[6]	NaClO ₄ ^[7]
	HT phase, stable above 581 K	Phase stable below 581 K
Chemical formula	NaClO ₄	NaClO ₄
Molecular weight [g mol ⁻¹]	122.44	122.44
Crystal system	Cubic	Orthorhombic
Space group	<i>Fm</i> $\bar{3}m$ (no. 225)	<i>Cmcm</i> (no. 63)
<i>a</i> [Å]	7.08	7.085(1)
<i>b</i> [Å]	7.08	6.526(1)
<i>c</i> [Å]	7.08	7.048(1)
α [°]	90	90
β [°]	90	90
γ [°]	90	90
<i>V</i> [Å ³]	354.89	325.88
<i>Z</i>	4	
ρ_{calc} [g cm ⁻³]		
<i>T</i> [K]	315 °C	

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Strontium nitrate

Name [German, acronym]: Strontium nitrate [strontiumnitrat]
Main (potential) use: Pyrotechnics, gas-generating propellants, airbags, tracer powder and red-colored flares^[4], component of illuminants^[4], pyrotechnic oxidizer and red flame color agent^[6], red fire in pyrotechnics, signal lights, marine signals, matches^[7]

Structural formula:



	Strontium nitrate	
Formula	$\text{Sr}(\text{NO}_3)_2$	
Molecular mass [g mol ⁻¹]	211.7	
Appearance at RT	White granules or powder ^[4, 7] , colorless crystals/white powder ^[6]	
N [%]	13.23	
Ω(CO ₂) [%]		
T _{m.p.} [°C]	570 ^[1, 4, 6, 7]	
T _{dec.} [°C]	618 (fusion), 672 (vigorous bubbling), 685 (slight nitrous fumes), 715 (rapid nitrous fumes) (DTA @ 15 °C/min) ^[3] , dec. on heating above mpt. ^[6]	
ρ [g cm ⁻³]	2.99 ^[1, 6, 7] , sp. gr. = 2.98 ^[4]	
Heat of formation	−4,622 kJ/kg (Δ _f H°) ^[1] , −978 kJ/mol (enthalpy of form.) ^[6]	
	Calcd. (EXPLO5 6.03)	Exptl.
−Δ _{ex} U° [kJ kg ⁻¹]		
T _{ex} [K]		
p _{C-J} [kbar]		
VoD [m s ⁻¹]		
V ₀ [L kg ⁻¹]		

Solubility [g/mL]	80 g/100 g in H ₂ O @ 25 °C ^[6] , soluble in 1.5 parts water ^[7] , slightly soluble in EtOH, acetone ^[7]
Hygroscopicity	Critical humidity = 86% RH @ 20 °C ^[5] , somewhat hygroscopic, can be dried in oven then protected from moist air ^[6]
Compatibility	Wet mixture with Al can result in exothermic reaction ^[6]
pH	Aqueous soln. is neutral ^[7]

	Strontium nitrate ^[2]
Chemical formula	$\text{Sr}(\text{NO}_3)_2$
Molecular weight [g mol^{-1}]	211.7
Crystal system	Cubic
Space group	$Pa\bar{3}$ (no. 205)
a [Å]	7.8220(10)
b [Å]	7.8220(10)
c [Å]	7.8220(10)
α [°]	90
β [°]	90
γ [°]	90
V [Å ³]	478.58(11)
Z	4
ρ_{calc} [g cm^{-3}]	
T [K]	173(2)

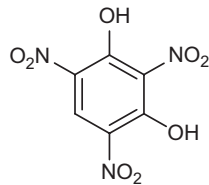
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Styphnic acid

Name [German, acronym]: Styphnic acid, 1,3-dihydroxy-2,4,6-trinitrobenzene, 2,4,6-trinitroresorcinol, 2,4,6-trinitrobenzene-1,3-diol, 2,4-dihydroxy-1,3,5-trinitrobenzene [trinitroresorcinol, styphninsäure, TNR]

Main (potential) use: Lead salt is used as primary explosive

Structural formula:



	TNR
Formula	C ₆ H ₃ N ₃ O ₈
Molecular mass [g mol ⁻¹]	245.10
Appearance at RT	Yellow crystalline solid ^[18, 19] , bright-yellow crystals (hexagonal) ^[26, 28] , becomes almost colorless on vacuum sublimation but turns yellow on contact with air ^[28]
IS [J]	7.4 Nm ^[10] , 10.54 ^[4] , 35% TNT ^[12] , same as PA ^[12] , <i>H</i> _{50%} = 43 cm ^[13, 17] , 43 cm (2.5 kg mass) ^[21] , 24.0 cm (2.5 kg mass, AFATL) ^[21] , <i>H</i> ₅₀ = 43 cm (2.5 kg mass, type 12 tool) ^[23] , log(<i>H</i> ₅₀) = 1.633 (<i>Kamlet/Adolph</i>) ^[24]
FS [N]	>353 ^[10]
ESD [J]	12.30 ^[5, 6] , 230.0 mJ ^[5] , 12.3 ^[29]
<i>N</i> [%]	17.14
Ω(CO ₂) [%]	−35.9
<i>T</i> _{m.p.} [°C]	175–176 ^[1] , 176 ^[10] , 176–177 (stable modification) ^[12] , 165–166 (unstable modification) ^[12] , 175.5 ^[18, 19, 28] , 176.2–176.5 ^[18] , 180 ^[26] , 179–180 ^[28]
<i>T</i> _{dec.} [°C]	223 (DSC @ 5 °C/min) ^[2]
ρ [g cm ⁻³]	2.012 (@ 293 K) ^[3] , 1.83 ^[10, 17] , sp. gr. = 1.83 ^[26]
Heat of formation	−523.0 kJ/mol (Δ _f <i>H</i> ^o), −2,133.8 kJ/kg (enthalpy of form.) ^[10] , −467.5 kJ/mol (based on Δ <i>H</i> _c) ^[14] , −111.7 kcal/mol (Δ _f <i>H</i> (s)) ^[17] , 404.8 kcal/kg ^[25]
Heat of combustion	−23,222.31 kJ/mol (bomb calorimetry) ^[14] , 2,310 kcal/kg (@ C ^v) ^[25]

	Calcd. (EXPLO5 5.04)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^{\circ}$ [kJ kg ⁻¹]	3,969	1.15 kcal/g (Q_{max} , calcd.) ^[17]	2,952 [H ₂ O (l)] ^[7, 10] 2,510 [H ₂ O (g)] ^[9] 2,843 [H ₂ O (g)] ^[10]
T_{ex} [K]	3,093		
$p_{\text{C-J}}$ [kbar]	237	263 (@ 1.83 g cm ⁻³) ^[17]	
VoD [m s ⁻¹]	7,522 (@ TMD)	7,660 (@ 1.83 g cm ⁻³) ^[17]	~50% MF ^[12]
V_0 [L kg ⁻¹]	622		814 ^[8]

Trauzl test [cm ³ , % TNT]	105–115% TNT ^[15] , 284 ^[27]																		
Sand test [g]	94% TNT ^[15]																		
Ballistic mortar test	108% TNT ^[15]																		
Initiation efficiency	<p>Minimum amount of primary explosive (g) needed for detonation (0.5 g Styphnic acid in No. 8 detonator shell, primary placed on top and compressed under reinforcing capsule @ 3,400 lb/in²): 0.110 g DDNP^[20], 0.225 g MF^[20], 0.075 g LA^[20], cap detonator causes it to explode^[26]</p> <p>Minimum amount of primary explosive (g) needed for detonation (0.4 g Styphnic acid, primary explosive, compressed in detonator capsule @ 1,000 lb/in²): 0.20 g fulminate with reinforcing cap^[20], 0.08 g HMTD (with reinforcing cap)^[20], 0.10 g HMTD (without reinforcing cap)^[20]</p>																		
5 s explosion T [°C] Explosion T [°C]	314 ^[12]																		
Thermal stability	Deflagrates on rapid heating ^[28]																		
Burn rate [mm/s]	Ignited TNR burns with bright flame without explosion ^[26]																		
Solubility [g/mL]	<p>Soluble in EtOH^[18], H₂O^[18], poorly soluble in water (bright yellow soln.): 0.65% dissolve in water @ 14 °C^[26] and 1.1% @ 62 °C^[26], 1 g in 156 mL H₂O @ 14 °C^[28], 1 g in 88 mL water @ 62 °C^[28], freely soluble in EtOH, Et₂O^[28] 0.641 g dissolves in 100 mL H₂O @ 14 °C^[18], 1.136 g dissolves in 100 mL H₂O @ 62 °C^[18], 0.45 dissolves in 100 mL H₂O @ 15 °C^[18], 0.55–0.58 g dissolves in 100 mL H₂O @ 20 °C^[18], 0.68–0.69 g dissolves in 100 mL H₂O @ 25 °C^[18]</p> <p>Solubility of styphnic acid in g in 100 g solvents @ T (°C)^[26]:</p> <table border="1"> <tr> <th>Solvent</th><th colspan="4">Solubility of styphnic acid (g) in 100 g Solvent @ T</th></tr> <tr> <td></td><td>0</td><td>5</td><td>10</td><td>17</td></tr> <tr> <td>Alcohol</td><td>5.10</td><td>–</td><td>–</td><td>6.22</td></tr> </table>				Solvent	Solubility of styphnic acid (g) in 100 g Solvent @ T					0	5	10	17	Alcohol	5.10	–	–	6.22
Solvent	Solubility of styphnic acid (g) in 100 g Solvent @ T																		
	0	5	10	17															
Alcohol	5.10	–	–	6.22															

	<table><tr><td>Benzene</td><td>–</td><td>4.5</td><td>–</td><td>–</td></tr><tr><td>Toluene</td><td>–</td><td>–</td><td>3.1</td><td>–</td></tr><tr><td>Acetone</td><td>–</td><td>–</td><td>–</td><td>313.1</td></tr></table>	Benzene	–	4.5	–	–	Toluene	–	–	3.1	–	Acetone	–	–	–	313.1
Benzene	–	4.5	–	–												
Toluene	–	–	3.1	–												
Acetone	–	–	–	313.1												
Hygroscopicity	Slightly hygroscopic ^[18] , absorbs 2–3% H ₂ O after exposure to atmosphere of 60% rel. hum. @ 25 °C for 30–100 h ^[19] , becomes almost colorless on vacuum sublimation but turns yellow on contact with air ^[28]															
Compatibility	Reacts with Cu, Sn Pb and Cd ^[26] , aqueous soln. dissolves Fe and Zn liberating hydrogen ^[26] , carbonates decompose TNR with liberation of CO ₂ ^[26] , dil. and conc. nitric or sulfuric acids do not react with TNR even on boiling ^[26] , reacts with aqua regia ^[26]															
Dipole moment [D]	1.78 (calcd.) ^[21]															
Acidity	Strong acid ^[26] , dibasic acid ^[26, 28] , acid to litmus ^[28]															
Δ <i>H</i> _{sub} [kJ/mol]	120.8 (exptl.) ^[22] , 123.4 (calcd., QSPR) ^[22]															

	Styphnic acid ^[11]
Chemical formula	C ₆ H ₃ N ₃ O ₈
Molecular weight [g mol ⁻¹]	245.10
Crystal system	Trigonal
Space group	<i>P</i> 3 c 1 (no. 158)
<i>a</i> [Å]	12.7
<i>b</i> [Å]	12.7
<i>c</i> [Å]	10
α [°]	90
β [°]	90
γ [°]	120
<i>V</i> [Å ³]	1,396.81
<i>Z</i>	6
ρ_{calc} [g cm ⁻³]	1.748
<i>T</i> [K]	295

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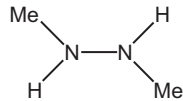
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Symmetrical dimethylhydrazine

Name [German, acronym]: *N,N'*-Dimethylhydrazine, *sym*-dimethylhydrazine, 1,2-dimethylhydrazine, hydrazomethane, dimethylhydrazine, symmetrical [1,2-dimethylhydrazin, SDMH]

Main (potential) use: liquid propellant

Structural formula:



	sym-DMH		
Formula	C ₂ H ₈ N ₂		
Molecular mass [g mol ⁻¹]	60.10		
Appearance at RT	Flammable, mobile liquid ^[1] , colorless liquid ^[2] , colorless liquid with ammonia smell ^[3]		
<i>N</i> [%]	46.62		
Ω(CO ₂) [%]	−212.98		
<i>T</i> _{m.p.} [°C]	−9 ^[3]		
<i>T</i> _{b.p.} [°C]	bp ₇₅₃ = 81 ^[1] , 87 (@ normal pressure) ^[2] , 81 (@ 1004 hPa) ^[3]		
<i>T</i> _{dec.} [°C]			
ρ [g cm ⁻³]	<i>d</i> ²⁰ ₄ = 0.8274 ^[1] , 0.83 (@ 20 °C) ^[3]		
Heat of formation			
Heat of combustion	−1,983.0 ± 4.2 kJ/mol (Δ _c <i>H</i> ^o , liq.) ^[4]		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
−Δ _{ex} <i>U</i> ^o [kJ kg ⁻¹]			
<i>T</i> _{ex} [K]			
<i>p</i> _{C-J} [kbar]			
VoD [m s ⁻¹]			
<i>V</i> ₀ [L kg ⁻¹]			
Vapor pressure [Pa]	70.8 hPa (@ 20 °C) ^[3]		
Volatility			
Burn rate [mm/s]			

Solubility [g/mL]	Miscible with water with release of large amounts of heat ^[1] , miscible with EtOH, Et ₂ O, DMF, hydrocarbons ^[1] , miscible with water ^[3]
Hygroscopicity	Hygroscopic – fumes in air and gradually turns yellow ^[1]
Photosensitivity	
Compatibility	Fumes in air and gradually turns yellow ^[1] , forms explosive mixtures with air ^[3]
Refractive index	$n_D^{20} = 1.4209$ ^[1]
Heat of vaporization [kJ/mol]	35.16 ^[2] , 35.16 (@ 360.2 K, $\Delta_{\text{vap}}H$) ^[4] , 41.0 (@ 286 K, $\Delta_{\text{vap}}H$) ^[4]
Heat of fusion [kJ/mol]	13.638 (@ 264.8 K) ^[4] , 13.64 (@ 264.3 K) ^[4]
Flash point [°C]	<5 ^[3]
Heat capacity, C_p [J/mol K]	171.04 (@ 298.15 K) ^[4]

- [1] *The Merck Index – An Encyclopedia of Chemicals and Drugs*, 9th edn., M. Windholz, S. Budavari, L. Y. Stroumtsos, M. N. Fertig (eds.), Merck and Co. Inc., Rahway, New Jersey, USA, **1976**.
- [2] V. Majer, V. Svoboda, *Enthalpies of Vaporization of Organic Compounds: A Critical Review and Data Compilation*, Blackwell Scientific Publications, Oxford, **1985**, p. 300.
- [3] *1,2-Dimethylhydrazin*, GESTIS-Stoffdatenbank des Institut für Arbeitsschutz der Deutschen Gesetzlichen Unfallversicherung, [http://gestis.itrust.de/nxt/gateway.dll/gestis_de/034110.xml?f=templates\\$fn=default.htm\\$3.0](http://gestis.itrust.de/nxt/gateway.dll/gestis_de/034110.xml?f=templates$fn=default.htm$3.0)
- [4] P. J. Lindstrom, W. G. Mallard, *NIST Chemistry WebBook*, NIST Standard Reference Database, National Institute of Standards and Technology, Gaithersburg, USA, webbook.nist.gov.

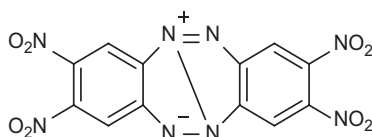
T

Tacot

Name [German, acronym]: Tacot, tetranitrodibenzo-1,3a,4,6a-tetrazapentalene, tetranitro-1,2,5,6-tetraazadibenzocyclooctatetraene, z-Tacot, 2,4,8,10-tetranitrobenzotriazolo[2,1-*a*]benzotriazol-6-ium inner salt (z-Tacot), (2,4,8,10-Tetranitrobenzotriazolo[1,2-*a*]bentotriazol-6-ium inner salt (y-Tacot), tetranitrobenzotriazolo [1,2-*a*]benzotriazole (t-Tacot))

Main (potential) use: Was used as grenade and mine filling, potential high thermal stability explosive, secondary explosive, useful when high-temperature resistance is required^[17], commercially available as flexible linear-shaped charges (FLSC), PBXs, high density charges and mild detonating fuzes^[17]

Structural formula:



	Tacot*
Formula	C ₁₂ H ₄ N ₈ O ₈
Molecular mass [g mol ⁻¹]	388.21
Appearance at RT	Orange solid ^[15] , orange-red crystals (commercial) ^[17]
IS [J]	69 Nm ^[4, 17] , 12 in (P.A.) ^[7] , 50% point >56 in (5 kg mass) ^[6] , 50% point = 102 cm (type 12 apparatus) ^[6] , H _{50%} = 66–89 cm ^[7] , H _{50%} = 101 cm ^[7, 13] , 69.0 (E _d , Bruceton method) ^[16] , 28 (ZBL-B instrument) ^[21]
FS [N]	50% point = 418 cm, no fires @ 440 cm ^[7] , >360 (FSKM 10 instrument) ^[21]
ESD [J]	No det. when 3 grains of unconfined loose charge subjected to 30,000 V discharge from 2,000 microfarad condenser ^[6] , 7 (ESD 2008A electric spark tester) ^[21]
N [%]	28.86
Ω(CO ₂) [%]	−74.2

$T_{m.p.}$ [°C]	378 ^[4, 22] , 378 (dec.) ^[6] , 410 ^[7] , >360 ^[1] , dec. without melting ^[17] , 400 (dec., y-Tacot) ^[22] , 398 (y-Tacot) ^[22]		
$T_{dec.}$ [°C]	Dec. >380 ^[5] , 354 (onset exotherm) ^[8, 18] , 381 (deflagration exotherm) (DTA) ^[8, 18] , 410 (single crystal, slow heating from ambient τ) ^[13] , 410 ^[15] , starts dec. @ 300 ^[15] , 368 (DTA, onset, exotherm) ^[16] , 378 (exo peak, DSC, z-TACOT) ^[17] , 400 (exo peak, DSC, y-TACOT) ^[17] , 401 ^[21]		
ρ [g cm ⁻³]	1.85 ^[4, 22] , 1.61 (nominal) ^[5] , 1.84 ^[6] , 1.84–1.86 (crystal) ^[13] , 1.76 (gas pycnometry @ 25 °C) ^[21] , 1.84 (calcd., y-Tacot) ^[22]		
Heat of formation	462.015 kJ/mol ($\Delta_f H^\circ$, EXPLO5 6.04), 536 kJ/mol ($\Delta_f H$) ^[5, 21] , 152 kcal/mol (standard enthalpy of form. @ 298 K (calcd.)) ^[17] , 465 kJ/mol (enthalpy of form. in (s)) ^[17] , 1,190.12 kJ/kg ($\Delta_f H^\circ$, EXPLO5 6.04), 1,380 kJ/kg ($\Delta_f H$) ^[5] , 1,188 kJ/kg ($\Delta_f H$, ICT thermochemical database) ^[14] , 459 kJ/mol ($\Delta_f H$) ^[24] , 111.0 kcal/mol ^[25] , 461.1 kJ/mol (enthalpy of form., exptl.) ^[26] , 460.7 kJ/mol (enthalpy of form., calcd., emp.) ^[26] , 315.4 kJ/mol (enthalpy of form., calcd., S-D method) ^[26]		
Heat of combustion	3,575 cal/g ^[6, 13] , 537 cal/mol ^[6]		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{ex}U^\circ$ [kJ kg ⁻¹]	4,534	141 kcal/g [H ₂ O (l)] (calcd. using $\Delta_f H$) ^[5] 135 kcal/g [H ₂ O (g)] (calcd. using $\Delta_f H$) ^[5] 4,121 (calcd., ICT-code, z-Tacot) ^[14] 4,374 MJ•kg ⁻¹ (Q_{real} , calcd., semi-empirical Pepekkin method, TACOT-Z) ^[16] 3,487 (@ 1.81 g cm ⁻³ , calcd., LOTUSES) ^[24]	4,103 [H ₂ O (l)] ^[4] 98 kcal/g [H ₂ O (l)] ^[5, 7] 96 kcal/g [H ₂ O (g)] ^[5]
T_{ex} [K]	3,383	3,086 (calcd., ICT-code, z-Tacot) ^[14] 3,900 (@ 1.81 g cm ⁻³ , calcd., LOTUSES) ^[24] 3,330 (@ 1.85 g cm ⁻³ , calcd. BKWR) ^[25] 4,040 (@ 1.85 g cm ⁻³ , calcd. BKWS) ^[25]	

p_{C-J} [kbar]	238	<p>181 (@ 1.61 g cm⁻³, Ruby code)^[5]</p> <p>103.6 MPa (calcd., ICT-code, z-Tacot)^[14]</p> <p>24.5 GPa (@ 1.76 g cm⁻³, calcd., K-J)^[21]</p> <p>202 (@ 1.84 g cm⁻³, calcd., y-Tacot)^[22]</p> <p>23.15 GPa (@ 1.81 g cm⁻³, calcd., LOTUSES)^[24]</p> <p>288 (@ 1.85 g cm⁻³, calcd. BKWR)^[25]</p> <p>253 (@ 1.85 g cm⁻³, calcd. BKWS)^[25]</p>	245 (@ 1.85 g cm ⁻³) ^[22]
VoD [m s ⁻¹]	<p>7,493 (@ 1.85 g cm⁻³, $\Delta_f H = 462.015$ kJ/mol)</p>	<p>7,050 (@ 1.85 g cm⁻³, calcd., R-P method)^[10]</p> <p>6,448 (@ 78% TMD)^[7]</p> <p>7,250 (@ 89% TMD)^[7]</p> <p>7,440 (@ TMD, calcd., K-J, z-TACOT)^[16]</p> <p>7,200 (@ 1.76 g cm⁻³, calcd., K-J)^[21]</p> <p>7,060 (@ 1.84 g cm⁻³, calcd., y-Tacot)^[22]</p> <p>7,050 (@ 1.81 g cm⁻³, calcd., LOTUSES)^[24]</p> <p>7,790 (@ 1.85 g cm⁻³, calcd. BKWR)^[25]</p> <p>7,620 (@ 1.85 g cm⁻³, calcd. BKWS)^[25]</p>	<p>7,250 (@ 1.64 g cm⁻³)^[4, 6, 16, 18]</p> <p>7,250 (@ 1.85 g cm⁻³)^[2, 5, 11, 25]</p> <p>6,935 (@ 1.58 g cm⁻³)^[7]</p> <p>6,530 (@ 1.61 g cm⁻³)^[9]</p> <p>6,600 (in Al sheaths)^[13]</p> <p>7,300 (pellet form)^[13]</p> <p>6,448 (@ 1.45 g cm⁻³, 78.8% TMD, rate stick method, VoD photographically measured)^[13]</p> <p>6,690 (@ 1.59 g cm⁻³, 86.5% TMD, wedge max. thickness = 12.7 mm, NOL wedge test)^[13]</p> <p>2,300 ft/s (@ 1.86 g/mL)^[15]</p> <p>7,200 (@ 1.85 g cm⁻³)^[22]</p>
V_0 [L kg ⁻¹]	585		

Critical diameter, d_c [cm]	3 mm (@ 1.45 g cm ⁻³ , 78.4% TMD) ^[12] Data from ^[20] : <table><tr><td>ρ_0 (g/cc)</td><td>% TMD</td><td>d_c (cm)</td></tr><tr><td>1.45</td><td>78.8</td><td>< 0.3</td></tr></table>					ρ_0 (g/cc)	% TMD	d_c (cm)	1.45	78.8	< 0.3																																																																																												
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Sand test [g]	88% PETN ^[6]																																																																																																						
Ballistic mortar test	96% TNT ^[6]																																																																																																						
SSGT [cm]	Small-scale gap (booster) sensitivity test ^[13, 17] : <table><tr><td rowspan="2">Pressed composition</td><td colspan="2">@ 93% TMD</td><td colspan="2">@ 95% TMD</td></tr><tr><td>DBg</td><td>Lucite gap (mils)</td><td>DBg</td><td>Lucite gap (mils)</td></tr><tr><td>TACOT</td><td>7.5</td><td>182</td><td>–</td><td>–</td></tr></table> $DB_g = 30 - 10 \log (\text{test gap}/\text{ref. gap})$ Sensitivity change with density ^[13] : <table><tr><td>Loading pressure (psi)</td><td>Density (g/cm³)</td><td>% TMD</td><td>DBg</td><td>Lucite gap in mils</td></tr><tr><td>4,000</td><td>1.1620</td><td>63.2</td><td>5.56</td><td>278</td></tr><tr><td>8,000</td><td>1.2809</td><td>69.1</td><td>5.64</td><td>273</td></tr><tr><td>16,000</td><td>1.4345</td><td>78.0</td><td>6.06</td><td>248</td></tr><tr><td>32,000</td><td>1.5928</td><td>86.6</td><td>6.70</td><td>214</td></tr><tr><td>64,000</td><td>1.6983</td><td>92.3</td><td>7.46</td><td>180</td></tr></table> TMD = 1.85 g/cm ³ , (1) = z-Tacot, TMD = no mixed response zone ^[19] : <table><tr><td rowspan="2">Loading pressure (kpsi)</td><td colspan="2">Density (g/cm³)</td><td rowspan="2">% TMD</td><td colspan="4">Sensitivity (DBg)</td></tr><tr><td>AVG.</td><td>S</td><td>AVG.</td><td>g</td><td>s_m</td><td>N</td></tr><tr><td>4</td><td>1.162</td><td>0.0139</td><td>62.8</td><td>5.562</td><td>0.0773</td><td>0.0434</td><td>20</td></tr><tr><td>8</td><td>1.281</td><td>0.0100</td><td>69.2</td><td>5.656</td><td>0.0911</td><td>0.0490</td><td>20</td></tr><tr><td>16</td><td>1.434</td><td>0.0074</td><td>77.5</td><td>6.050</td><td></td><td></td><td>20 (1)</td></tr><tr><td>32</td><td>1.593</td><td>0.0046</td><td>86.1</td><td>6.705</td><td>0.0788</td><td>0.0444</td><td>20</td></tr><tr><td>64</td><td>1.698</td><td>0.0100</td><td>91.8</td><td>7.487</td><td>0.1520</td><td>0.0932</td><td>20</td></tr></table>					Pressed composition	@ 93% TMD		@ 95% TMD		DBg	Lucite gap (mils)	DBg	Lucite gap (mils)	TACOT	7.5	182	–	–	Loading pressure (psi)	Density (g/cm ³)	% TMD	DBg	Lucite gap in mils	4,000	1.1620	63.2	5.56	278	8,000	1.2809	69.1	5.64	273	16,000	1.4345	78.0	6.06	248	32,000	1.5928	86.6	6.70	214	64,000	1.6983	92.3	7.46	180	Loading pressure (kpsi)	Density (g/cm ³)		% TMD	Sensitivity (DBg)				AVG.	S	AVG.	g	s_m	N	4	1.162	0.0139	62.8	5.562	0.0773	0.0434	20	8	1.281	0.0100	69.2	5.656	0.0911	0.0490	20	16	1.434	0.0074	77.5	6.050			20 (1)	32	1.593	0.0046	86.1	6.705	0.0788	0.0444	20	64	1.698	0.0100	91.8	7.487	0.1520	0.0932	20
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5 s explosion T [°C] 15 min explosion T [°C] Ignition T [°C]	337 ^[6] 388–400 ^[6] ~494 ^[8] , ignites in 15 min @ 337 ^[13] , ignites in 0.1 s between 388 and 400 ^[13] , 374 ^[16] , ~497 ^[18]																																
Thermal stability [°C]	Begins autocatalysis in 15 min @ 300 ^[13] , thermally stable @ 280 for ≥ 2 h ^[13] , 300 °C (threshold of thermal stability) ^[16]																																
Vacuum stability test [cm ³ /h]	0.04–0.08 mL/g/48 h @ 120 °C ^[7] , 0.1 mL/g/h @ 260 °C ^[7] , 0.3 mL/g/h @ 280 °C ^[7] , 0.0 cc/g/48 h @ 100 °C ^[13] , 0.7 cc/g/h @ 260 °C (average for 2 h exposure) ^[13] , 2.0 cc/g/h @ 280 °C (average for 2 h exposure) ^[13] t-TACOT @ 200 °C, total gas evolved (cm ³ /g) @ STP/time of exposure (days) ^[14] : 0.1/2, 0.5/7, 0.9/14, 1.3/21, 1.6/28, 1.9/35, 2.1/42, 2.5/49, 3.0/56, 3.5/63, 3.9/70, 4.3/77, 4.8/84, 5.3/91 ^[14, 23] z-TACOT @ 200 °C, total gas evolved (cm ³ /g) @ STP/time of exposure (days) ^[14] : 0.4/2, 0.6/7, 0.7/14, 0.8/21, 1.0/28, 4.1/35, 4.9/42, 7.1/49, 8.6/56, 10.8/63, 11.2/70, 11.4/77, 11.5/84, 11.5/91 ^[14] z-TACOT @ 175 °C, total gas evolved (cm ³ /g) @ STP/time of exposure (days) ^[23] : 0.4/2, 0.5/7, 0.6/14, 0.7/21, 0.8/28, 0.8/35, 0.8/42, 0.8/49, 0.8/56, 0.9/63, 1.0/70, 1.1/77, 1.4/84, 1.7/91 ^[23]																																
Specific heat capacity, C_p [kcal/mol]	Calcd. values for gaseous TACOT ^[17] : <table><tr><td>T (K)</td><td>C_p (kcal/mol)</td><td>T (K)</td><td>C_p (kcal/mol)</td></tr><tr><td>300</td><td>52.5</td><td>2,000</td><td>114.4</td></tr><tr><td>400</td><td>64.4</td><td>2,500</td><td>116.5</td></tr><tr><td>500</td><td>74.2</td><td>3,000</td><td>117.8</td></tr><tr><td>600</td><td>81.9</td><td>3,500</td><td>118.7</td></tr><tr><td>800</td><td>92.9</td><td>4,000</td><td>119.2</td></tr><tr><td>1,000</td><td>100.1</td><td>4,500</td><td>119.6</td></tr><tr><td>1,500</td><td>109.7</td><td>5,000</td><td>119.9</td></tr></table>	T (K)	C_p (kcal/mol)	T (K)	C_p (kcal/mol)	300	52.5	2,000	114.4	400	64.4	2,500	116.5	500	74.2	3,000	117.8	600	81.9	3,500	118.7	800	92.9	4,000	119.2	1,000	100.1	4,500	119.6	1,500	109.7	5,000	119.9
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300	52.5	2,000	114.4																														
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800	92.9	4,000	119.2																														
1,000	100.1	4,500	119.6																														
1,500	109.7	5,000	119.9																														
Solubility [g/mL]	Soluble in acetone ^[15] , recryst. from acetone (γ -Tacot) ^[22] , insoluble (<0.1 g/100 mL solvent) in CHCl ₃ , EtOH, H ₂ O ^[5] , slightly soluble (0.1–5 g/100 mL solvent) in DMFA, DMSO, nitric acid, pyridine ^[5]																																

Processing	Vacuum pressing of pure Tacot pellets ½ in diameter × ½ in long @ 20,000 psi ^[13] :						
	T (°C)	Dwell (min)	Ejection T (°C)	Results	Density (g/cm ³)	% TMD	Solvent
	150	20	50	Cracked	–	–	None
	140	20	50	Good	1.56	85.0	None
	150	20	25	Cracked	1.56	85.0	None
	50	30	25	Good	1.72	93.5	3% methylene chloride
	60	30	25	Good	1.75	95.0	3% acetone
	60	45	25	Cracked	–	–	3% acetone
	50	45	25	Good	1.76	95.5	3% acetone

Radiation sensitivity	Data from ^[27] :		
	Exposure rate (R/h)	Total dose (R)	Vacuum stability test
			200 °C (cc/2 g/2 h)
	8.5 × 10 ⁵	Control	0.10
		1.4 × 10 ⁷	0.27
		1.2 × 10 ⁸	0.14
		1.1 × 10 ⁹	0.51
		3.7 × 10 ⁹	2.44
	DTA for irradiated explosives @ 20 °C/min ^[27] :		
	Total dose (R)	Exotherms	
		First	
		Onset (°C)	Peak (°C)
	0	340	376
0	365	398	
1.4 × 10 ⁷	365	398	
1.2 × 10 ⁸	350	398	
1.1 × 10 ⁹	350	385	
3.7 × 10 ⁹	320	387	

TGA for irradiated explosives^[27]:

Total dose (R)	Heating rate (°C/min)	Weight (mg)	Start of dec (°C)	10% weight loss T (°C)	Total weight loss (%)	Remarks
0	20	8.4	350	—	7 @ 406 °C	Detonated @ 406 °C
1.4×10^7	20	7.2	340	—	7 @ 287 °C	Detonated @ 387 °C
1.2×10^8	20	9.7	320	—	8 @ 372 °C	Detonated @ 372 °C
1.1×10^9	20	9.9	320	—	9 @ 387 °C	Detonated @ 387 °C
3.7×10^9	20	8.5	240	354	18 @ 370 °C	Detonated @ 370 °C
7.0×10^9	20	10.75	180	330	17 @ 355 °C	Detonated @ 355 °C

Effect of gamma radiation on the mpt. and color^[27]:

Total dose (R)	mpt. (°C)	Color
0	390 dec.	Red orange
1.4×10^7	390 dec.	Red orange
1.2×10^8	388 dec.	Brownish orange
1.1×10^9	378 dec.	Reddish dark brown
3.7×10^9		Maroon dark brown

IS for irradiated explosives, 50% fire height in inches, Bruceton method (P.A. apparatus, 2 kg mass)^[27]:

Total Co ⁶⁰ gamma dose (R)	\bar{X} mean (in)	σ std. dev. (in)
0	12.0	1.86
1.4×10^7	12.5	1.34
1.2×10^8	12.32	1.25
1.1×10^9	11.83	2.28

Effect of gamma radiation on explosion T (5 s explosion T in °C) and activation energy (kcal/mol)^[27]:

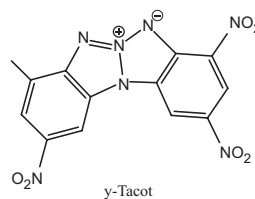
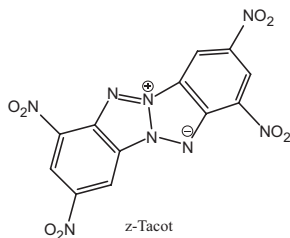
Total dose (R)	5 s explosion T (°C)	Apparent activation energy (kcal/mol)
0	415	31.14
1.4×10^7	411	26.16
1.2×10^8	407	26.58
1.1×10^9	404	27.50

Effect of gamma radiation on rates of detonation^[27]:

Total dose (R)	Density (g/cc)	Density after irradiation (g/cc)	Rate of detonation (m/s)	Detonation pressure (kbar)
0	1.58	—	6,935	190
1.1×10^7	1.57	1.57	6,915	188
1.3×10^8	1.56	1.56	6,910	186
1.1×10^9		1.38	6,285	136

* Du Pont: Tacot is usually a mixture of isomers of the $-\text{NO}_2$ groups, but since the properties are similar, the isomers are not usually separated^[8]

† Two Tacot isomers have been isolated: z and y , the values given in this section are for z -Tacot unless otherwise stated^[22]:



- [1] M. S. Chang, R. R. Orndoff, *Method for the Preparation of Tetranitrodibenzo-tetrazapentalene*, US Patent 4,526,980A, **1985**.
- [2] M. H. Keshavarz, *J. Haz. Mat.*, **2009**, 166, 762–769.
- [3] M. H. Keshavarz, *Propellants, Explosives, Pyrotechnics*, **2012**, 37, 489–497.
- [4] R. Meyer, J. Köhler, A. Homburg, *Explosives*, Wiley-VCH, Weinheim, **2016**, pp. 230–233.
- [5] B. M. Dobratz, *Properties of Chemical Explosives and Explosive Simulants*, UCRL-5319, LLNL, December 15 **1972**.

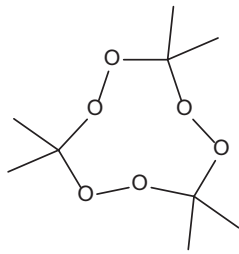
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TATP

Name [German, acronym] Triacetonetriperoxide, tricycloacetone peroxide, acetone peroxide trimer, 3,3,6,6,9,9-hexamethyl-1,2,4,5,7,8-hexaoxocyclononane, 3,3,6,6,9,9-hexamethyl-1,2,4,5,7,8-hexanone, peroxyacetone [TATP, APEX]

Main (potential) use: Improvised explosive, patented as primary charge for detonators (not used due to its low mpt. and ease of sublimation)^[19], suggested as component for secondary explosives^[19], no current industrial or military use^[19]

Structural formula:



	TATP		
Formula	C ₉ H ₁₈ O ₆		
Molecular mass [g mol ⁻¹]	222.24		
Appearance at room temperature (RT)	Colorless crystals (cubes) ^[19] , white solid on grinding ^[19] , colorless solid ^[21] , white crystalline substance with an acid odor which readily sublimates at RT ^[29] , white crystalline solid ^[31]		
IS [J]	1.5 (<100 μm), 0.3 (BAM) ^[1, 4, 5] , 0.03 kg ^[7] , 0.03 kg (0/6 positive results, BAM) ^[7]		
	Material ^[19]	Impact energy (J) ^[19]	Drop-height (2 kg mass, cm) ^[19]
	TATP fine powder	3.1	16
	TATP small crystals	2.4	12
	TATP and 20% glass rubble	1.0	5
	TATP and 8–10% oil	4.3–5.5	22–28

	<p>0.1 (resublimed TATP)^[21], 0.5 (crude TATP from aqueous synthesis)^[21], 1.5 (1/6 positive, BAM)^[21], 6.5 cm^[23], 0.3 Nm^[24, 25], Fol = <10 (below sensitivity threshold of machine, Rotter impact test, 30 mg sample, 5 kg mass)^[24], 0.5 (hydrated TATP, ~ 20%, 50% GO)^[27], 0.1 (anhydrous (sublimed) TATP, 50% GO)^[27]</p> <p>Gelled TATP with different TATP concentrations and different gels, CGC = critical gellator concentration, BAM, Bruceton method, $E_{50\%}$^[28]: TATP (no gel), powdered, 6 J^[28]; TATP = 21% v/v, GSSG gellant system, DMF solvent, 8.2 mM CGC, 30 J^[28]; TATP = 24.4% v/v, sol–gel system (% v/v) = 50 TEOS, 30 MTES, 20 DDES, $f_n = 3.219$, >49 J^[28]; TATP = 35.8% v/v, sol–gel system (% v/v) = 50 TEOS, 30 MTES, 20 DDES, $f_n = 3.219$, >49 J^[28]; TATP = 23.9% v/v, sol–gel system (% v/v) = 60 TEOS, 20 MTES, 20 DDES, $f_n = 3.313$, >49 J^[28]; TATP = 35.2% v/v, sol–gel system (% v/v) = 60 TEOS, 20 MTES, 20 DDES, $f_n = 3.313$, >49 J^[28]</p> <p>10 tests per sample, up-down method, ERL apparatus^[29]:</p> <table><tr><th>Material</th><th>Impact energy (J)^[29]</th><th>T (°C)/RH (%)</th></tr><tr><td>TATP needle-like crystals</td><td>< 1.2</td><td>21/74</td></tr><tr><td>TATP fine powder</td><td>< 2.0</td><td>18/27</td></tr><tr><td>TATP fine powder</td><td>1.9</td><td>19/26</td></tr><tr><td>TATP crystals</td><td>< 1.2</td><td>17/25</td></tr><tr><td>TATP fine powder</td><td>2.3</td><td>19/28</td></tr></table>	Material	Impact energy (J) ^[29]	T (°C)/RH (%)	TATP needle-like crystals	< 1.2	21/74	TATP fine powder	< 2.0	18/27	TATP fine powder	1.9	19/26	TATP crystals	< 1.2	17/25	TATP fine powder	2.3	19/28
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TATP fine powder	1.9	19/26																	
TATP crystals	< 1.2	17/25																	
TATP fine powder	2.3	19/28																	
FS [N]	<p><5 (<100 μm), 0.1^[1, 4, 5], 1.6 N^[3], extremely sensitive^[6], <0.01 kgf^[7], <0.5 kgf (below detection limit of apparatus, BAM)^[7], 0.05 (resublimed TATP)^[21], 0.2 (crude TATP from aqueous synthesis)^[21], <5 (1/6 positive, BAM)^[21], 39^[23], <0.1 N^[24], <5 N (below threshold of machine, BAM)^[24], 0.1^[25], 25 (hydrated TATP, ~20%, 2.5 kg, 50% GO, steel against steel)^[27], 0.2 (hydrated TATP, ~20%, 20 g, 50% GO, porcelain against porcelain)^[27], 0.2 (anhydrous (sublimed) TATP, 20 g, 50% GO, steel against steel)^[27], <0.05 (anhydrous (sublimed) TATP, 5 g, 50% GO, minimal load with mini-BAM apparatus, porcelain against porcelain)^[27]</p>																		

Gelled TATP with different TATP concentrations and different gels, CGC = critical gellator concentration, BAM, Bruceton method, $E_{50\%}$ [28]:

Gel type	Gellant system	Solvent	CGC	TATP conc. [% v/v]	FS [N]
–	–	Powdered	–	100	6
Physical organic gels	GSSG	DMF	8.2 mM	21	7
	Sylvagel-1000	EG	3.3% w/v	31	6
		EGME	2.0% w/v	16	192
				33	144
				44	122
Physical hydrogels	Guar gum	H ₂ O	0.035 m/mL	13	360
		H ₂ O/EtOH		16	360
	Xanthan gum	H ₂ O/EtOH	0.120 g/mL	23	360
	1.5% w/w PAA	H ₂ O/ isopropanol	Not a solid gel	35	16
	3.0% w/w PAA			35	16
	Physical cross-linked hydrogel (ionotropic gel)			33	14

FS of TATP in hybrid silicon-based gels at different TATP concentrations and in different gels, BAM, Bruceton method, $E_{50\%}$ [28]:

Sol-gel system (% v/v)			f_n	TAP conc. (% v/v)	FS (N)
TEOS	MTES	DDES			
50	20	30	3.098	26	10
50	30	20	3.219	23.2	> 360
				24.3	324
				24.4	20
				35.8	20
60	20	20	3.313	22.9	324
				23.2	360
				23.7	84
				23.9	16
				35.2	12
				57.1	12

	TATP FS, 10 tests per sample, up-down method, Julius-Peters BAM apparatus ^[29] : <table><tr><th>Material</th><th>Friction (kp/cm²)^[29]</th><th><i>T</i> (°C)/ RH (%)</th></tr><tr><td>TATP needle-like crystals</td><td>< 1.0</td><td>21 / 74</td></tr><tr><td>TATP fine powder</td><td>< 0.5</td><td>18 / 27</td></tr><tr><td>TATP fine powder</td><td>< 0.5</td><td>19 / 26</td></tr><tr><td>TATP crystals</td><td>< 0.5</td><td>17 / 25</td></tr><tr><td>TATP fine powder</td><td>< 0.5</td><td>19 / 28</td></tr></table>	Material	Friction (kp/cm ²) ^[29]	<i>T</i> (°C)/ RH (%)	TATP needle-like crystals	< 1.0	21 / 74	TATP fine powder	< 0.5	18 / 27	TATP fine powder	< 0.5	19 / 26	TATP crystals	< 0.5	17 / 25	TATP fine powder	< 0.5	19 / 28
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TATP crystals	< 0.5	17 / 25																	
TATP fine powder	< 0.5	19 / 28																	
ESD [J]	0.2 (<100 μm), 0.16 ^[1, 5] , 0.0056 ^[4] , <i>E</i> ₅₀ = 160 mJ (pure TATP) ^[19] , 0.2 (<100 μm, OZM ESD 2010 EN) ^[21] , 0.006 ^[23] , <0.045 (below threshold sensitivity of machine, DSTO apparatus) ^[24]																		
<i>N</i> [%]	0																		
Ω(CO ₂) [%]	−151.2																		
<i>T</i> _{m.p.} [°C]	<p>97–98 (measured on Buechi device); 80 (endotherm peak), 120 (exotherm peak) (DSC @ 20 °C/min, pure TATP; DSC is highly dependent on purity of the TATP; TATP samples show endotherm peak in range 80–140 and exotherm peak in range 120–240)^[7], 98 (DSC @ 20 °C/min)^[8], 95^[4], 16.5% sublimed within 48 h^[15], 95–98.8^[19], 97–98 (@ 5 °C/min, glass capillary)^[21], 91^[25], 94^[29], 92–93^[29], 95–97 (sealed in capillary tubes, @ 3 °C/min, Boitus mpt. apparatus)^[31], 97.4 (onset), 98.2 (peak max) (DSC @ 10 K/min, N₂, Al pan with pierced lid)^[33]</p> <p>DSC (monoclinic <i>P</i>₂₁/<i>c</i>, <i>a</i> = 13.788(6) crystals): first cycle of heating (up to 120 °C @ 1 °C/min): 95.5–96.5 (endotherm, sublimation, onset <i>T</i> = 95.0), cooling gas back to 50 °C (cooling rate = 5 °C/min) 67–68 (exotherm, solidification, onset <i>T</i> = 67.7), heating this solid again 89–90 (resublimation, onset <i>T</i> = 87.8)^[9]</p> <p>DSC (monoclinic <i>P</i>₂₁/<i>c</i>, <i>a</i> = 11.964(2) crystals): first cycle of heating (up to 120 °C @ 1 °C/min): 93.6 (endotherm, sublimation, onset), cooling gas back to 50 °C (cooling rate = 5 °C/min) 65.9 (exotherm, solidification, onset), heating this solid again 88.1 (resublimation, onset)^[9]</p> <p>DSC (monoclinic <i>P</i>₂₁/<i>c</i>, <i>a</i> = 11.968(2) crystals): first cycle of heating (up to 120 °C @ 1 °C/min): 94.7 (endotherm, sublimation, onset), cooling gas back to 50 °C (cooling rate = 5 °C/min) 64.8 (exotherm, solidification, onset), heating this solid again 88.1 (resublimation, onset)^[9]</p> <p>DSC (monoclinic <i>P</i>₂₁/<i>c</i>, <i>a</i> = 11.9620(6) crystals): first cycle of heating (up to 120 °C @ 1 °C/min): 91.6 (endotherm, sublimation, onset), cooling gas back to 50 °C (cooling rate = 5 °C/min) 63.1 (exotherm, solidification, onset), heating this solid again 88.3 (resublimation, onset)^[9]</p>																		
<i>T</i> _{phase transition} [°C]	86 (phase 1b→ phase 1a) (DSC @ 2 °C/min, crimped Al pan) ^[22]																		

$T_{\text{dec.}}$ [°C]	<p>150–160^[1, 5, 29], 80 (endotherm peak), 120 (exotherm peak) (DSC @ 20 °C/min, pure TATP DSC is highly dependent on purity of the TATP; TATP samples show endotherm peak in range 80–140 and exotherm peak in range 120–240)^[7], 215 (range of ~ 80 °C, broad exotherm, DSC @ 20 °C/min)^[8], >150–160^[19], >160 (onset, DSC @ 10 °C/min, recryst. TATP, sealed pan)^[19]</p> <p>Dependence of dec. onset on acetone:acid molar ratio (n_c/n_a, using acid as catalyst, heating rate = 5 °C/min)^[19]:</p> <table><tr><th>Molar ratio ($n_c:n_a$)</th><th>Acid = H₂SO₄</th><th>Acid = HClO₄</th><th>Acid = HCl</th><th>Acid = HNO₃</th></tr><tr><td>$2.5\text{--}5 \times 10^{-1}$</td><td>Dec. onset before melting</td><td>Dec. starts before melting</td><td>Dec. starts > 145 °C</td><td>Dec. starts > 145 °C</td></tr><tr><td>1×10^{-1} $\text{--}5 \times 10^{-2}$</td><td>Dec. during melting</td><td>Dec. during melting</td><td></td><td></td></tr><tr><td>1×10^{-2} $\text{--}2.5 \times 10^{-4}$</td><td>Dec starts > 145 °C</td><td>Dec. starts > 145 °C</td><td></td><td></td></tr></table>	Molar ratio ($n_c:n_a$)	Acid = H ₂ SO ₄	Acid = HClO ₄	Acid = HCl	Acid = HNO ₃	$2.5\text{--}5 \times 10^{-1}$	Dec. onset before melting	Dec. starts before melting	Dec. starts > 145 °C	Dec. starts > 145 °C	1×10^{-1} $\text{--}5 \times 10^{-2}$	Dec. during melting	Dec. during melting			1×10^{-2} $\text{--}2.5 \times 10^{-4}$	Dec starts > 145 °C	Dec. starts > 145 °C																	
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$T_{\text{sublimation}}$ [°C]	<p>94 (endo, DSC @ 2 °C/min, crimped Al pan)^[22]</p> <p>DSC transition temperatures, heating rate of 1 °C/min, run at T range 50–120 °C, cooling cycle run from 120 to 50 °C at a rate of 5 °C/min^[9]:</p> <table><tr><th>Polymorph</th><th>1a</th><th>1d</th><th>1e</th><th>1f</th></tr><tr><td>First heating cycle onset T (°C)</td><td>95.0</td><td>93.6</td><td>94.7</td><td>91.6</td></tr><tr><td>$\Delta H_{\text{sublimation}}$ (J/g)</td><td>96.5</td><td>65.8</td><td>101.1</td><td>347.4</td></tr><tr><td>First cooling cycle onset T (°C)</td><td>67.7</td><td>65.9</td><td>64.8</td><td>63.1</td></tr><tr><td>$\Delta H_{\text{sublimation}}$ (J/g)</td><td>80.9</td><td>62.4</td><td>47.6</td><td>212.7</td></tr><tr><td>Second heating cycle onset T (°C)</td><td>87.8</td><td>88.1</td><td>88.1</td><td>88.3</td></tr><tr><td>$\Delta H_{\text{sublimation}}$ (J/g)</td><td>73.2</td><td>52.0</td><td>40.4</td><td>168.0</td></tr></table>	Polymorph	1a	1d	1e	1f	First heating cycle onset T (°C)	95.0	93.6	94.7	91.6	$\Delta H_{\text{sublimation}}$ (J/g)	96.5	65.8	101.1	347.4	First cooling cycle onset T (°C)	67.7	65.9	64.8	63.1	$\Delta H_{\text{sublimation}}$ (J/g)	80.9	62.4	47.6	212.7	Second heating cycle onset T (°C)	87.8	88.1	88.1	88.3	$\Delta H_{\text{sublimation}}$ (J/g)	73.2	52.0	40.4	168.0
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ρ [g cm ^{–3}]	1.272 (@ 180 K), 1.250 (calcd.), 1.18 ^[1, 5] , 1.272 ^[4] , 1.272 (X-ray) ^[19, 21, 25] , 1.25 (@ 298 K, calcd.) ^[21] , 1.004 ^[29]																																			
Heat of formation	–583.8 kJ/mol (ΔH_f°) ^[1, 4] , 583.5 kJ/mol (ΔH_f° ₂₉₈ , exptl., (g)) ^[16] , –640 kJ/mol (ΔH_f° , calcd., CBS-4M) ^[21] , 90.8 kJ/mol ^[19] , –2,804.5 kJ/kg (enthalpy of form.) ^[25] , –90.8 kJ/mol (enthalpy of form.) ^[31] , 151.4 ± 32.7 kJ/mol (enthalpy of form., ΔH_{f298}° , semi-micro oxygen bomb calorimetry) ^[31] , –395 kJ/mol (enthalpy of form., est. by semi-empirical AM1 with allowance for heat of sublimation) ^[31] , –561.8 ± 51.0 kJ/mol (ΔH_f° ₂₉₈ (gas), calcd., G4 method, average value from isodesmic and atomization reactions) ^[31] , –664.5 ± 44 kJ/mol (ΔH_f° ₂₉₈) ^[31] , –583.8 ± 44 kJ/mol (ΔH_f° ₂₉₈ (gas), exptl.) ^[31] , –132.4 kcal/mol (ΔH_f° (gas), calcd.) ^[25] , –622.6 kJ/mol (ΔH_f° (s), calcd.) ^[25] , –90.8 kJ/mol (enthalpy of form., $\Delta_f H^\circ$ ₂₉₈) ^[16] , 151.4 kJ/mol ($\Delta_f H^\circ$ ₂₉₈ , exptl., semi-micro bomb calorimetry) ^[16] , 151.4 ± 32.7 kJ/mol ($\Delta_f H^\circ$) ^[33]																																			

Heat of combustion	2,405 kJ/kg (calcd.) ^[16] , $-\Delta_c H = 5,449.7 \pm 44$ kJ/mol ^[31] , 2,405 kJ/kg (heat of combustion, calcd. from measured flame T) ^[31] , $-\Delta U_c = 24,507 \pm 199$ J/g or $5,446 \pm 44$ kJ/mol (exptl., bomb calorimeter) ^[31] , $\Delta_c U^\circ = -28,177 \pm 147$ J/g ^[33] , $\Delta_c U^\circ = -6,261.8 \pm 32.7$ kJ/mol ^[33] , $\Delta_c H^\circ = -6,265.5 \pm 32.7$ kJ/mol ^[33]		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{\text{ex}} U^\circ$ [kJ kg ⁻¹]	3,420 (@ 1.25 g cm ⁻³ , $\Delta H_f^\circ = -640$ kJ/mol) ^[21]	2,745 ^[1, 4, 5] 5,665 (heat of explosion, <i>Muraour</i> , but cited in ^[31] as being too high) ^[31]	5,665 (small pressed sample) ^[16] 2,803 (cast, small pressed sample) ^[16, 31] 2,745 (heat of explosion, @ 0.42 g cm ⁻³ load ρ , 1.20 g sample, Al shell, bomb calorimeter) ^[31]
T_{ex} [K]	2,038 (@ 1.25 g cm ⁻³ , $\Delta H_f^\circ = -640$ kJ/mol) ^[21]	2,895 (@ 100% TMD, calcd., Cheetah-6) ^[20]	
p_{C-J} [kbar]	114 (@ 1.25 g cm ⁻³ , $\Delta H_f^\circ = -640$ kJ/mol) ^[21]	132 (@ 100% TMD, calcd., Cheetah-6) ^[20]	
VoD [m s ⁻¹]	6,322 (@ 1.25 g cm ⁻³ , $\Delta H_f^\circ = -640$ kJ/mol) ^[21]	5,300 (@ 1.18 g cm ⁻³) ^[1, 4-6, 17]	5,290 (@ 1.2 g cm ⁻³ , detonated in column, 6.3 mm diameter) ^[6] 3,065 (@ 0.68 g cm ⁻³ , detonated in column, 15 mm diameter) ^[6] 3,750 (@ 0.92 g cm ⁻³) ^[6] 5,300 (@ 1.18 g cm ⁻³) ^[1, 4, 19] 1,430 (@ 0.47 g cm ⁻³ , initiated by pyroxylin layer, steel confinement) ^[15, 19] 3,750 ^[15] 3,950 ^[15] 3,950 (@ 0.95 g cm ⁻³) ^[19]
V_0 [L kg ⁻¹]	821 (@ 1.25 g cm ⁻³ , $\Delta H_f^\circ = -640$ kJ/mol) ^[21]	855 ^[4, 5]	855 (@ 0.42 g cm ⁻³ load ρ , 1.20 g sample, Al shell, bomb calorimeter) ^[31]

Trauzl test [cm ³ , % TNT]	250 cc (10 g TATP, cf. 285 cc for TNT) ^[6] , 80% TNT ^[29]																																
Sand test [g]	80% TNT ^[17] , 34.1 g sand crushed by 0.4 g initiated by 0.2 g MF (cf. 48.0 g with TNT) ^[6] , 250 cc (10 g TATP, cf. 300 cm ³ for TNT) ^[11] , 71% TNT ^[19] , 46.2–50.5% TNT ^[19]																																
Initiation efficiency	TATP and acceptor both pressed under 25 MPa: 0.05 g initiates PETN ^[19] , 0.09 g initiates Tetryl ^[19] , 0.16 g initiates TNT ^[19]																																
Dead-pressing	Dead-pressed @ 49 MPa ^[19]																																
5 s explosion <i>T</i> [°C] Ignition <i>T</i> [°C]	Sublimes before reaction ^[24]																																
Thermal stability	Spectroscopically pure TATP samples produced using aq. HCl as catalyst and which have been recryst. several times from MeOH did not show any transformation to DADP after 4 weeks @ RT in contrast to TATP produced using sulfuric acid ^[33]																																
Vapor pressure [atm. @ °C]	24.8 Pa @ 25 °C ^[14] , 6.95 Pa (gas chromatography) ^[19] , 7.87 Pa (@ 25 °C, gas chromatography) ^[19] Values from ^[30] , cited in ^[29] : <table><tr><td><i>T</i> (K)</td><td>Vapor pressure (Pa)</td><td><i>T</i> (K)</td><td>Vapor pressure (Pa)</td></tr><tr><td>285</td><td>0.95</td><td>305</td><td>18.9</td></tr><tr><td>285</td><td>1.13</td><td>315</td><td>46.1</td></tr><tr><td>295</td><td>1.85</td><td>315</td><td>51.2</td></tr><tr><td>295</td><td>1.44</td><td>325</td><td>98.4</td></tr><tr><td>298</td><td>6.95</td><td>325</td><td>101</td></tr><tr><td>298</td><td>6.86</td><td>331</td><td>720</td></tr><tr><td>305</td><td>16.8</td><td>331</td><td>596</td></tr></table>	<i>T</i> (K)	Vapor pressure (Pa)	<i>T</i> (K)	Vapor pressure (Pa)	285	0.95	305	18.9	285	1.13	315	46.1	295	1.85	315	51.2	295	1.44	325	98.4	298	6.95	325	101	298	6.86	331	720	305	16.8	331	596
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298	6.95	325	101																														
298	6.86	331	720																														
305	16.8	331	596																														
Volatility	~66% mass lost in 2 weeks @ RT ^[11] , ~6.5% mass lost in 2 weeks @ RT ^[6, 18] , 68.6% mass lost in 14 days @ RT ^[6, 18] , 1.5% mass lost in 2 h @ 50 °C ^[6, 18] , 100% mass lost in 3 h @ 50 °C ^[6] Sublimation: 6.5% (by mass) within 48 h @ 18 °C ^[24]																																
Heat of sublimation [kJ/mol]	72.5 (calcd., Clapeyron eqn.) ^[19] , 80.6 (calcd., <i>Egorshév</i>) ^[19] , 80.7 ^[31]																																
Heat of evaporation [kJ/mol]	58.1 (calcd., <i>Egorshév</i>) ^[19] , enthalpy of vaporization = 40.39 ± 3.0 kJ/mol ^[29] , enthalpy of vaporization = 46.41 kJ/mol ^[29] , enthalpy of vaporization = 51.73 kJ/mol ^[29]																																
Heat of melting [kJ/mol]	22.6 (calcd., <i>Egorshév</i>) ^[19]																																

Burn rate [mm/s]	Dependence of burn rate on pressure ^[19] :																																				
	<table><tr><th>Pressure (MPa)^[19]</th><th>Burn rate (mm s⁻¹)^[19]</th><th>Pressure (MPa)^[19]</th><th>Burn rate (mm s⁻¹)^[19]</th></tr><tr><td>~0.017</td><td>~ 1.7</td><td>~ 0.75</td><td>~ 35</td></tr><tr><td>~0.03</td><td>~ 3.3</td><td>~ 1.1</td><td>~ 50</td></tr><tr><td>~0.045</td><td>~ 4.9</td><td>~ 2.1</td><td>~ 80</td></tr><tr><td>~0.07</td><td>~ 8</td><td>~ 3.5</td><td>~ 100</td></tr><tr><td>~0.1</td><td>~ 10</td><td>~ 10</td><td>~ 300</td></tr><tr><td>~0.2</td><td>~ 18</td><td>~ 18</td><td>~ 450</td></tr></table>	Pressure (MPa) ^[19]	Burn rate (mm s ⁻¹) ^[19]	Pressure (MPa) ^[19]	Burn rate (mm s ⁻¹) ^[19]	~0.017	~ 1.7	~ 0.75	~ 35	~0.03	~ 3.3	~ 1.1	~ 50	~0.045	~ 4.9	~ 2.1	~ 80	~0.07	~ 8	~ 3.5	~ 100	~0.1	~ 10	~ 10	~ 300	~0.2	~ 18	~ 18	~ 450								
	Pressure (MPa) ^[19]	Burn rate (mm s ⁻¹) ^[19]	Pressure (MPa) ^[19]	Burn rate (mm s ⁻¹) ^[19]																																	
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	~0.1	~ 10	~ 10	~ 300																																	
~0.2	~ 18	~ 18	~ 450																																		
Linear and mass rates of burning @ 1 atm ^[32] : $u = 0.95 \text{ cm/s}$ ^[32] , $m = 1.16 \text{ g cm}^{-2} \text{ s}^{-1}$ ^[32]																																					
Solubility [g/mL]	Insoluble in H ₂ O, aq. NH ₃ ^[19] , soluble in most common organic solvents ^[19] , soluble in toluene ^[25] , soluble in acetone ^[25] , 3.1 g/L in H ₂ O @ 25 °C ^[29] , recryst. from hot MeOH ^[33]																																				
	Solubility in g/100 mL solvent ^[19] :																																				
	<table><tr><th>Solvent</th><th>@ 17 °C</th><th>@ RT</th></tr><tr><td>Acetone</td><td>7.96</td><td>16.5</td></tr><tr><td>Benzene</td><td>19.3</td><td>–</td></tr><tr><td>CS₂</td><td>11.2</td><td>–</td></tr><tr><td>CCl₄</td><td>52.5</td><td>–</td></tr><tr><td>CHCl₃</td><td>110</td><td>111</td></tr><tr><td>Et₂O</td><td>4.2</td><td>–</td></tr><tr><td>EtOH</td><td>0.12</td><td>3.5</td></tr><tr><td>Hexane</td><td>–</td><td>11.1</td></tr><tr><td>MeOH</td><td>–</td><td>3.8</td></tr><tr><td>Pyridine</td><td>17.9</td><td>–</td></tr><tr><td>Toluene</td><td>–</td><td>34.7</td></tr></table>	Solvent	@ 17 °C	@ RT	Acetone	7.96	16.5	Benzene	19.3	–	CS ₂	11.2	–	CCl ₄	52.5	–	CHCl ₃	110	111	Et ₂ O	4.2	–	EtOH	0.12	3.5	Hexane	–	11.1	MeOH	–	3.8	Pyridine	17.9	–	Toluene	–	34.7
	Solvent	@ 17 °C	@ RT																																		
	Acetone	7.96	16.5																																		
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	Toluene	–	34.7																																		
	mL solvent required to dissolve 100 mg TATP @ RT ^[26] : 1.0 (acetone) ^[26] , 3.0 (Diesel) ^[26] , 1.2 (ethyl acetate) ^[26] , 2.1 (<i>i</i> -octane) ^[26] , 0.8 (toluene) ^[26] , 3.0 (EtOH, 100%) ^[26] , 62.2 (EtOH, 50%) ^[26] , 3.8 (<i>i</i> -PrOH) ^[26] , 40.2 (<i>i</i> -PrOH, 50%) ^[26] , 14–16 ppm (H ₂ O) ^[26] , very poor solubility in H ₂ O ^[26]																																				
Solubility in ionic liquids @ 25 °C, TATP concentration wt. % ^[27] : 0.4% in 3MBP BF ₄ , 0.5% in HP BF ₄ , 1.0 in HP Tf ₂ N, 1.0 in EMIM C ₈ H ₁₇ OSO ₃ , 1.25 in DMIM BF ₄ , 2.2 in OMIM BF ₄ , 1.3 in HMIM BF ₄ , 0.1 in EMIM BF ₄ , 0.8 in HMIM Tf ₂ N, 0.9 in BMIM Tf ₂ N, 0.3 in EMIM Tf ₂ N ^[27]																																					

Hygroscopicity	Nonhygroscopic ^[19]																																				
Compatibility	TATP reacts violently with conc. H ₂ SO ₄ ^[26]																																				
	TATP destruction tests, methods for TATP dec. (destruction) ^[26] :																																				
	<table><tr><th>Mass TATP (g)</th><th>Solvent</th><th>Solvent (mL)</th><th>Acid</th><th>Acid (mL)</th><th>Time to destruction</th></tr><tr><td>100</td><td>EtOH 50%</td><td>200</td><td>HCl 36%</td><td>400</td><td>20 min</td></tr><tr><td>100</td><td>IPA 50%</td><td>200</td><td>HCl 36%</td><td>400</td><td>20 min</td></tr><tr><td>100</td><td>IPA 50%</td><td>100</td><td>HCl 36%</td><td>400</td><td>2 h 20 min</td></tr><tr><td>460</td><td>IPA 50%</td><td>900</td><td>HCl 36%</td><td>425</td><td>25 min</td></tr></table>	Mass TATP (g)	Solvent	Solvent (mL)	Acid	Acid (mL)	Time to destruction	100	EtOH 50%	200	HCl 36%	400	20 min	100	IPA 50%	200	HCl 36%	400	20 min	100	IPA 50%	100	HCl 36%	400	2 h 20 min	460	IPA 50%	900	HCl 36%	425	25 min						
	Mass TATP (g)	Solvent	Solvent (mL)	Acid	Acid (mL)	Time to destruction																															
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460	IPA 50%	900	HCl 36%	425	25 min																																
DDT	Transition distance = 1.7 mm, 30–50% TMD ^[23]																																				
Activation energy to dec. [kcal/mol]	36.3 (thermal dec. of TATP in soln. @ 150–230 °C) ^[25]																																				
Heat of dec. [kJ kg ^{−1}]	>3,765 (calcd. from dec. products @ low heating rates) ^[31] , 4,853 (calcd. from dec. products @ fast heating rates) ^[31] , 2,261 (isothermal dec., based on exptl. Δ <i>H</i> _f) ^[31] , 2,285 (fast temperature rise, based on exptl. Δ <i>H</i> _f) ^[31]																																				
Δ <i>H</i> _{sub} [kcal/mol]	16.4 ^[25]																																				
Max. combustion <i>T</i> [°C]	1,300 K (measured using thin thermocouples) ^[31]																																				
Brisance	Brisance: (30 mm Al witness plate, No. 8 detonator, stainless steel cylinder, 10 mm diameter, 35 mm high, standard prEN 13,763-15 test setup), ρ (TATP) = 1.26 g cm ^{−3} , mass of TATP = 2.27 g, manufacturing pressure = 720 bar, dent depth = 3.65 mm ^[7] . Overall brisance range of TATP is 60–100% TNT (standard No. 8 detonator dent depth = 1.96 mm) ^[7]																																				
	<table><tr><th>TATP^[7] (ρ/g cm^{−3})</th><th>Mass TATP (g)</th><th>Diameter (mm)</th><th>Manufacturing pressure (bar)</th><th>Effect</th><th>Dent depth (mm)</th></tr><tr><td>0.86</td><td>1.14</td><td>7.62</td><td>Manually</td><td>Detonation</td><td>2.5</td></tr><tr><td>1.03</td><td>1.54</td><td>7.65</td><td>303.5</td><td>Detonation</td><td>2.03</td></tr><tr><td>1.18</td><td>1.35</td><td>7.7</td><td>~ 425</td><td>Low order detonation</td><td>0.26</td></tr><tr><td>1.18</td><td>1.69</td><td>7.65</td><td>607</td><td>Low order detonation</td><td>0.3</td></tr><tr><td>1.25</td><td>2.29</td><td>10.20</td><td>720</td><td>Deflagration (burn)</td><td>-</td></tr></table>	TATP ^[7] (ρ/g cm ^{−3})	Mass TATP (g)	Diameter (mm)	Manufacturing pressure (bar)	Effect	Dent depth (mm)	0.86	1.14	7.62	Manually	Detonation	2.5	1.03	1.54	7.65	303.5	Detonation	2.03	1.18	1.35	7.7	~ 425	Low order detonation	0.26	1.18	1.69	7.65	607	Low order detonation	0.3	1.25	2.29	10.20	720	Deflagration (burn)	-
	TATP ^[7] (ρ/g cm ^{−3})	Mass TATP (g)	Diameter (mm)	Manufacturing pressure (bar)	Effect	Dent depth (mm)																															
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1.25	2.29	10.20	720	Deflagration (burn)	-																																

	TATP ^[10,29]	TATP ^[111]	TATP ^[12]	TATP ^[9]	TATP ^[9]	TATP ^[9]	TATP ^[9]	TATP ^[9]	TATP ^[13]	TATP ^[13]	TATP ^[9]
Chemical formula	C ₉ H ₁₈ O ₆	C ₉ H ₁₈ O ₆	C ₉ H ₁₈ O ₆	C ₉ H ₁₈ O ₆	C ₉ H ₁₈ O ₆	C ₉ H ₁₈ O ₆	C ₉ H ₁₈ O ₆	C ₉ H ₁₈ O ₆	C ₉ H ₁₈ O ₆	C ₉ H ₁₈ O ₆	C ₉ H ₁₈ O ₆
Molecular weight [g mol ⁻¹]	222.23	222.23	222.23	222.23	222.23	222.23	222.23	222.23	222.23	222.23	222.23
Crystal system	Monoclinic	Monoclinic	Monoclinic	Orthorhombic	Triclinic	Monoclinic	Monoclinic	Monoclinic	Triclinic	Monoclinic	Monoclinic
Space group	<i>P</i> 2 ₁ / <i>c</i> (no. 14)	<i>P</i> 2 ₁ / <i>c</i> (no. 14)	<i>P</i> 2 ₁ / <i>c</i> (no. 14)	<i>Cmca</i> (no. 64)	<i>P</i> $\bar{1}$ (no. 2)	<i>P</i> 2 ₁ / <i>c</i> (no. 14)	<i>P</i> 2 ₁ / <i>c</i> (no. 14)	<i>P</i> 2 ₁ / <i>c</i> (no. 14)	<i>P</i> $\bar{1}$ (no. 2)	<i>P</i> 2 ₁ / <i>c</i> (no. 14)	<i>P</i> 2 ₁ / <i>c</i> (no. 14)
<i>a</i> [Å]	13.925(5)		13.7617(7)	28.055(4)	8.901(1)	11.964(2)	11.968(2)	11.9620(6)	8.900(2)	13.8088(12)	13.788(6)
<i>b</i> [Å]	10.790(4)		10.6514(6)	15.616(6)	10.500(2)	28.083(6)	14.029(3)	14.0380(4)	10.997(2)	10.6956(7)	10.664(5)
<i>c</i> [Å]	7.970(4)		7.8800(4)	10.667(1)	12.576(1)	15.600(3)	15.606(3)	15.5950(8)	12.569(3)	7.8949(7)	7.894(4)
α [°]	90	90	90	90	82.560(9)	90	90	90	82.587(6)	90	90
β [°]	91.64(5)	91.77(5)	91.8240(10)	90	84.445(7)	117.22(3)	117.15(3)	117.270(2)	84.276(6)	91.635(7)	91.77(5)
γ [°]	90	90	90	90	73.053(6)	90	90	90	73.014(6)	90	90
<i>V</i> [Å ³]	1,197.01	1,160.1(9)	1,154.48(11)	4,673.3(2)	1,112.7(3)	4,660.9(15)	2,331.5(8)	2,327.7(18)	1,164.1(5)	1,165.55(16)	1,160.1(9)
<i>Z</i>	4	4	4	16	4	16	4	4	4	4	4
ρ_{calc} [g cm ⁻³]	1.233	1.272	1.279	1.263	1.327	1.267	1.266	1.268	1.268	1.266	1.272
<i>T</i> [K]	295	180	120	200	200	200	200	200	200	193	180
		Crystals from slow sublimation in closed flask @ RT		Polymorph 1b, prisms	Polymorph 1c, plates	Polymorph 1d	Polymorph 1e	Polymorph 1f			Polymorph 1a, needles

TATP forms ≥ 6 polymorphic crystals^[19]; raw TATP has three different crystal forms: needles (monoclinic), prisms (orthorhombic), plates (triclinic)^[19], crystallization from organic solvents results in another 3 orthorhombic crystalline forms^[19]; Crystallizations from the reaction solution always produced mixtures of polymorphs rather than a phase-pure sample^[9, 22]. Phase 1a is the most stable polymorph, all other polymorphs (1b–1f) transform spontaneously into phase 1a on standing as a consequence of the ready sublimation of TATP at room temperature and its subsequent crystallization on cooling^[22]. Phase 1b is kinetically favored phase, phase 1a is the thermodynamic phase^[22]. Powder X-ray diffraction patterns show the polymorph components of as-synthesized TATP samples, prepared using different routes^[22]:

TATP phase(s) from PXRD	Conditions	Factors influencing pure phase vs. mixed phase samples
Pure phase 1b	<p>TATP produced from percarbonate route, TATP produced from urea route, Hydrochloric acid and aq. H_2O_2; rapid crystallization</p> <ul style="list-style-type: none"> – Na_2CO_3, H_2O_2, HCl – urea, H_2O_2, HCl – urea, H_2O_2, H_2SO_4 – urea, H_2O_2, HNO_3 – aq. H_2O_2, HCl 	Acidity of soln., presence of carbonate ions or urea, ionic strength of soln.; high acid content, high ionic strength of soln., high concentrations of very strong acids, rapid crystallization favors phase pure phase 1b
Mixed phases	<p>Slow crystallization</p> <ul style="list-style-type: none"> – aq. H_2O_2, H_3PO_4 – aq. H_2O_2, HCl 	Lower ionic strength, lower acid concentration, weaker acids even in high concentrations, slow crystallization conditions favors formation of mixed phases
Almost pure phase 1a	Use of Lewis acid (e.g., SnCl_4)	Lewis acid acts as catalyst

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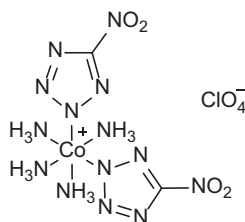
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Tetraamine-*cis*-bis(5-nitro-2*H*-tetrazolato) cobalt(III) perchlorate

Name [German, acronym]: Tetraamine-*cis*-bis(5-nitro-2*H*-tetrazolato) cobalt(III) perchlorate, tetraammine-bis-(5-nitrotetrazolato-*N*²) cobalt(III) perchlorate, bis-(5-nitro-2*H*- tetrazolato-*N*²) tetraamino cobalt perchlorate [BNCP]

Main (potential) use: Primary explosive, hot wire DDT designs^[4], possible substitute for LA^[4], safe commercial detonators^[5], primary or secondary charge in blasting caps^[5], pyrotechnic, automatic control systems of rockets^[5], energy producing component for semi-conducting bridge (SCB) initiator applications^[6]

Structural formula:



	BNCP
Formula	$\text{C}_2\text{ClCoH}_{12}\text{N}_{14}\text{O}_8$
Molecular mass [g mol ⁻¹]	454.59
Appearance at RT	Yellow-orange prismatic crystals ^[2] , light orange needle-shaped crystals ^[6]
IS [J]	30 cm ^[3] , 100 kg·cm ^[4] , $H_{50} = 30$ cm (2 kg mass) ^[6]
FS [N]	3 kg ^[3] , 0.6–1 kg (BAM) ^[4] , 3.0 kg (friction insensitiveness) ^[6]
ESD [J]	5 (spark insensitivity) ^[3] , >25 (Sandia Man Model testers) ^[4] , ~5 (spark insensitivity) ^[6]
N [%]	43.14
$\Omega(\text{CO}_2)$ [%]	
$T_{\text{dec.}}$ [°C]	269 ^[1, 5] , 260 ^[3]
ρ [g cm ⁻³]	2.03, 2.05 (@ 291 K) ^[1] , 2.031 (gas pycnometer) ^[2] , 2.03 (crystal) ^[5] , 0.3 (bulk density of crystals without additives) ^[6] , 0.6 (bulk density, increased by addition of 1% dextrin and dioctyl succinate during synthesis) ^[6]
Heat of formation	

	Calcd. (EXPLO5 6.03)	Exptl.
$-\Delta_{\text{ex}}U^{\circ}$ [kJ kg ⁻¹]		
T_{ex} [K]		
$p_{\text{C-J}}$ [kbar]		
VoD [m s ⁻¹]		Will detonate in column lengths (2–3 mm) in steel confinement) ^[4] 7,120 (@ 1.79 g cm ⁻³) ^[5]
V_0 [L kg ⁻¹]		

Ignition ability	Minimal charge in a No. 8 detonator toward RDX = 0.05 g ^[5] , BNCP and BNCP/NHN could not be initiated by flash and hot wire stimuli ^[6] , BNCP with CCP/NCP co-initiators could be initiated by flash and hot wire stimuli ^[6]		
5 s explosion T [°C] Explosion T [°C] Autoignition T [°C]	260 ^[6] 270 (DSC @ 10 °C/min, sealed hermetic pans and cups) ^[4]		
Thermal stability	Functional after exposure to 160 °C for 100 h ^[4]		
Compatibility	Compatible with all typical hot wire and EBW materials of construction ^[4] , compatible with epoxy adhesives ^[4]		
Witness plate dents	0.66 mm (steel witness plate) ^[4]		
	Performance evaluation of BNCP in detonator no. 27 ^[6] :		
	Composition quantity given in mg in brackets	Puncture on witness plate* diameter of the hole (mm)	Remarks
	BNCP (150) + LA (200)	No puncture	No initiation
	BNCP (150) + NHN (200)	No puncture	No initiation
	BNCP (150) + NCP/CCP (200)	9	Initiated
	BNCP (175) + NCP/CCP (175)	9	Initiated
	BNCP (200) + NCP/CCP (150)	9	Initiated
	BNCP (225) + NCP/CCP (125)	9	Initiated
	BNCP (250) + NCP/CCP (100)	9	Initiated
	BNCP (275) + NCP/CCP (75)	9	Initiated

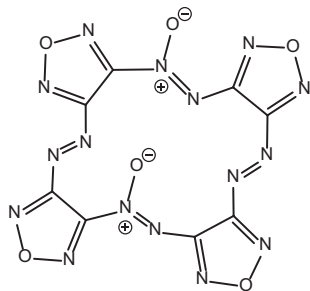
	BNCP (300) + NCP/CCP (50)	9	Initiated
	BNCP (325) + NCP/CCP (25)	9	Initiated
	NCP/CCP (350)	9	Initiated
	BNCP (325), NCP (25) and Tetryl/PETN (550)	9	Initiated
	BNCP (150), NCP (200) and Tetryl/PETN (550)	9	Initiated
	ASA composition (standard)	9	Initiated
LA = lead azide, SA = silver azide, CCP = cobalt carbohydrazide perchlorate, NCP = Nickel carbohydrazide perchlorate; ASA composition = service LA (SLA 65%), lead styphnate (LS 32.5%) and Al (2.5%); * each experiment was repeated five times to prove the reproducibility in detonator No. 27.			
Flying plate velocity [mm/μs]	3.2 ^[4]		
Time of DDT	10 μs ^[5]		
Heat of dec. [J/g]	3,319 (DSC) ^[5]		

	BNCP ^[2]	BNCP ^[2]
Chemical formula	C ₂ H ₁₂ ClCoN ₁₄ O ₈	C ₂ H ₁₂ ClCoN ₁₄ O ₈
Molecular weight [g mol ⁻¹]	454.59	454.59
Crystal system	Monoclinic	Monoclinic
Space group	<i>P</i> 2 ₁ / <i>n</i> (14)	<i>P</i> 2 ₁ / <i>n</i> (14)
<i>a</i> [Å]	10.031(2)	9.946(7)
<i>b</i> [Å]	10.547(2)	10.542(5)
<i>c</i> [Å]	14.861(3)	14.820(7)
α [°]	90	90
β [°]	109.09(3)	108.68(4)
γ [°]	90	90
<i>V</i> [Å ³]	1,485.8(6)	1,472.0(15)
<i>Z</i>	4	4
ρ_{calc} [g cm ⁻³]	2.032	2.051
<i>T</i> [K]	293	213

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3,4:7,8:11,12:15,16-Tetrafurazano-1,2,5,6,9,10,13,14-octaazacyclohexadeca-1,3,5,7,9,11,13,15-octane-1,10-dioxide

Name [German, acronym]: [DOATF]
Main (potential) use: under research
Structural formula:



	DOATF		
Formula	C ₈ N ₁₆ O ₆		
Molecular mass [g mol ⁻¹]	416.19		
Appearance at RT	Orange crystals ^[1]		
IS [J]	<i>H</i> _{50%} = 11.2 cm (2.5 kg mass, LANL type 12 test, Bruceton method) ^[1]		
FS [N]	4.7 kg (BAM, Bruceton, 50% load) ^[1]		
ESD [J]	0.125 (ABL) ^[1]		
<i>N</i> [%]	53.85		
Ω(CO ₂) [%]	−38.44		
<i>T</i> _{m,p.} [°C]	127 (DSC @ 10 °C/min, hermetically sealed Al pans with pinhole lid, 1 mg sample) ^[1] , 93 (Chinese value) ^[1] , 144 (Russian value) ^[1]		
<i>T</i> _{phase transition} [°C]			
<i>T</i> _{dec.} [°C]	212 (exo, onset), 289 (exo, peak max.) (DSC @ 10 °C/min, hermetically sealed Al pans with pinhole lid, 1 mg sample) ^[1]		
ρ [g cm ⁻³]	1.809 (X-ray, calcd. @ 113 K), 1.761 (X-ray, calcd. @ 293 K)		
Heat of formation			
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.

$-\Delta_{\text{ex}}U^\circ$ [kJ kg ⁻¹]			
T_{ex} [K]			
$p_{\text{C-J}}$ [kbar]		292 ^[1]	
VoD [m s ⁻¹]		8,200 ^[1]	
V_0 [L kg ⁻¹]			
Solubility [g/mL]	Crystals grown from hot toluene ^[1]		
Energy of dec. [J/g]	3,089 ^[1]		

	DOATF^[1]
Chemical formula	C ₈ N ₁₆ O ₆
Molecular weight [g mol ⁻¹]	416.24
Crystal system	Triclinic
Space group	<i>P</i> -1
<i>a</i> [Å]	5.7364(2)
<i>b</i> [Å]	11.5088(5)
<i>c</i> [Å]	12.0378(5)
α [°]	96.1030(10)
β [°]	98.3090(10)
γ [°]	101.1660(10)
<i>V</i> [Å ³]	764.08(5)
<i>Z</i>	2
ρ_{calc} [g cm ⁻³]	1.809 (calcd. @ 113 K) 1.761 (calcd. @ 293 K)
<i>T</i> [K]	113

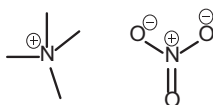
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Tetramethylammonium nitrate

Name [German, acronym]: Tetramethylammonium nitrate, nitetra
[tetramethylammoniumnitrat, Tetra-Salz, TeMeAN]

Main (potential) use: Was used as fuel component in fusible ammonium
nitrate mixtures^[4], acts as a fuel when mixed with
oxygen carriers^[5]

Structural formula:



	Tetramethylammonium nitrate
Formula	$C_4H_{12}N_2O_3$
Molecular mass [g mol ⁻¹]	136.2
Appearance at RT	White or colorless crystals ^[5] , white crystals ^[7]
IS [J]	No explosions @ 3 m (10 kg mass, encapsulated samples) ^[5] , attempts to provoke explosive dec. by impact failed ^[7]
N [%]	20.57
$\Omega(CO_2)$ [%]	-129.2
$T_{\text{phase transitions}}$ [°C]	DSC @ 20 K/min, 6 mg sample ^[6] : $\text{Phase-III} \xrightleftharpoons[290 \text{ K}]{292 \text{ K}} \text{Phase-II} \xrightleftharpoons[295 \text{ K}]{300 \text{ K}} \text{Phase-I}$
$T_{\text{m.p.}}$ [°C]	410 ^[1] , 326–328 (Ger.) ^[5] , 405–410 (Fr.) ^[5] , 410 ^[7]
$T_{\text{dec.}}$ [°C]	Color change @ 400 °C (heating in test tube from 250 °C @ 5 °C/min) ^[5]
ρ [g cm ⁻³]	1.25 ^[4, 5, 7] , 0.70 (bulk) ^[5] , 1.23 (cryst., measured) ^[6] , 1.22 (compressed under 3,400 kg/cm ²) ^[7]
Heat of formation	-330.4 kJ/mol ($\Delta_f H^\circ$) ^[2] , -2,507.3 kJ/kg (enthalpy of form.) ^[4] , -624 cal/g ^[3] , -607.4 kcal/kg (ΔH_f) ^[5] , 75.8 kcal/mol (@ 18 °C, F^V) ^[5] , 80.8 kcal/mol (@ 18 °C, F^P) ^[5] , -341.5 kJ/mol (enthalpy of form., exptl.) ^[8] , -337.5 kJ/mol (enthalpy of form., calcd., emp.) ^[8]
Heat of combustion	707.2 kcal/mol (@ 18 °C, Q_c^V) [H ₂ O (l)] ^[5]

	Calcd. (EXPLO5 6.03)	Exptl.
$-\Delta_{\text{ex}}U^{\circ}$ [kJ kg ⁻¹]	3,128	
T_{ex} [K]	1,952	
$p_{\text{C-J}}$ [kbar]	133	
VoD [m s ⁻¹]	6,745	
V_0 [L kg ⁻¹]	952	

Critical diameter [cm] [†]						
Trauzl test [cm ³ , % TNT] [†]	Could not be detonated when used alone ^[5] , 96cc (cf. 100 cc for PA if 50/50 mixture of TeMeAN/RDX used) ^[5] , 112.5 cc (cf. 100 cc for PA, 13.5% TeMeAN in mixture with AN and RDX) ^[5] , 119.5 cc (cf. 100 cc for PA, 13.5% TeMeAN in mixture with AN and 13% RDX) ^[5]					
Sand test [g] [†]						
Ballistic mortar test [†]						
Initiation efficiency	Does not detonate, even when initiated by a strong charge of PETN ^[7]					
Gap test	1.5 cm (13.5% TeMeAN in mixture with AN and RDX) ^[5] , 4.5 cm (11.7% TeMeAN in mixture with 13% RDX and AN) ^[5]					
LSGT [cm]	†					
SSGT [cm]	†					
Thermal stability	Color change to light brown @ ~ 400 °C and white smoke with sample converting to black liq. @ 410 °C (0.1 g sample, heated in test tube from 250 °C @ 5 °C/min) ^[5] , nitrous fumes produced and sample eventually turned black @ 370 °C after 2 min (sample immersed in metal bath) ^[5]					
Solubility [g/mL]	Soluble in hot water ^[5] , slightly soluble in cold water ^[5] , soluble in H ₂ O ^[7]					
Hygroscopicity	Less than AN ^[5]					
Compatibility	Incompatible with TNT ^[5]					
Flame sensitivity	On exposure to open flame, ignited after 50–60 s when placed in 20 mm × 1 m trough and burned with orange flame ^[5]					
Compressibility	Data from ^[5] :					
	Pressure (kg/cc)	68	170	270	850	3,400
	ρ (g/cc)	0.90	1.17	1.20	1.21	1.22
pK _a	pH = 7.0–7.1 (aq. soln.) ^[5]					

[†] Me₄N⁺NO₃⁻ has no explosive properties^[7]

	Tetramethylammonium nitrate ^[6]
Chemical formula	C ₄ H ₁₂ N ₂ O ₃
Molecular weight [g mol ⁻¹]	136.2
Crystal system	Tetragonal
Space group	<i>P4/nmm</i>
<i>a</i> [Å]	8.072(2)
<i>b</i> [Å]	
<i>c</i> [Å]	5.642(3)
α [°]	
β [°]	
γ [°]	
<i>V</i> [Å ³]	367.6
<i>Z</i>	2
ρ_{calc} [g cm ⁻³]	1.23
<i>T</i> [K]	303

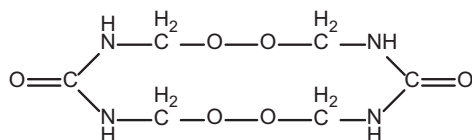
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Tetramethylene diperoxide dicarbamide

Name [German, acronym]: 1,2,8,9-Tetraoxa-4,6,11,13-tetraazacyclo-tetradecane-5,12-dione [TMDD]

Main (potential) use: Improvised explosive, suggested as component of priming mixtures in past to increase combustibility of the mixture^[1], primary explosive for blasting caps^[1, 5], patented as sensitizer for other explosives^[6], no widespread military or commercial use^[3]

Structural formula:



	TMDD
Formula	$C_6H_{12}N_4O_6$
Molecular mass [g mol ⁻¹]	236.18
Appearance at RT	White crystals ^[1] , white powder ^[2] , fine colorless needles ^[3]
IS [J]	Fol = 20 (average gas evolution = 1 mL; cf. RDX Fol = 80, Rotter impact apparatus, 20 mg sample, 2 kg mass) ^[3] , requires strong hammer blow to initiate explosion ^[4] , detonates reliably if 0.5 in steel ball of 8.3 g dropped from height of 12 in but no detonations if dropped from 5 in ^[5] , 30 in (50% ignition point, 2 kg mass) ^[6]
FS [N]	48 (10 mg sample, low report, barely audible cracking sound, Julius Peters BAM) ^[3] , initiation failed @ 42 N (Julius Peters BAM) ^[3]
ESD [J]	0.45 ^[3] , failed to initiate with 0.045 J ^[3] , amenable to electrical ignitions of 0.28–0.33 A ^[5]
N [%]	23.72
$\Omega(CO_2)$ [%]	−81.29
$T_{m.p.}$ [°C]	~180 ^[1]
$T_{dec.}$ [°C]	154.0 (exo, onset), 185.5 (exo, peak max) (DSC @ 5 °C/min) ^[3]
ρ [g cm ⁻³]	
Heat of formation	

	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^\circ$ [kJ kg ⁻¹]			
T_{ex} [K]			
$p_{\text{C-J}}$ [kbar]			
VoD [m s ⁻¹]			
V_0 [L kg ⁻¹]			
Temperature of ignition (°C)	162 (popping sound, test tube remained unbroken @ 5 °C/min) ^[3] , explosion with bright bang on rapid heating ^[4]		
Vapor pressure [atm. @ °C]	Extremely low ^[2]		
Solubility [g/mL]	Insoluble in H ₂ O, MeOH, EtOH, CHCl ₃ , pyridine, other common organic solvents ^[1] , minimal solubility/insoluble in most organic solvents ^[2] , soluble in sulfuric acid ^[2] , insoluble in a wide range of solvents ^[3]		
Heat of decomposition [J/g]	820 (exo dec. @ 185.5 °C, DSC) ^[3]		

	TMDD ^[3]
Chemical formula	C ₆ H ₁₂ N ₄ O ₆
Molecular weight [g mol ⁻¹]	236.20
Crystal system	Monoclinic
Space group	<i>Pc</i> (7)
<i>a</i> [Å]	4.587(4)
<i>b</i> [Å]	16.080(2)
<i>c</i> [Å]	6.690(5)
α [°]	90
β [°]	107.44(5)
γ [°]	90
<i>V</i> [Å ³]	470.8(5)
<i>Z</i>	2
ρ_{calc} [g cm ⁻³]	1.666
<i>T</i> [K]	100

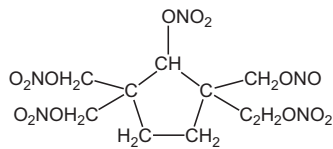
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2,2,5,5-Tetramethylcyclopentanol pentanitrate

Name [German, acronym]: Nitropentanol, tetramethylolcyclopentanol pentanitrate, nitrocyclopentanone, cyclopentanone pentanitrate [FIVOLITE]

Main (potential) use: melt-cost

Structural formula:



	Fivolite		
Formula	C ₉ H ₁₃ N ₅ O ₁₅		
Molecular mass [g mol ⁻¹]	431.23		
Appearance at RT	Solid ^[2] , pale pink solid (crude) ^[5] , granular solid, almost pink-free (pure) ^[5] , white crystalline solid (recryst.) ^[5]		
IS [J]	<i>H</i> _{50%} = 26 cm (2 kg mass) ^[1] , <i>H</i> _{50%} = 95 cm (similar to RDX) ^[5] , <i>H</i> ₅₀ = 29 cm (design no. 3 apparatus) ^[7]		
FS [N]	Less sensitive than RDX in sliding friction test ^[5] , 50% firing position = no firing @ 150 cm (6 lb sliding weight, 30° incline, RDX = 40 cm) ^[5] , slight crackling on vigorous grinding in unglazed porcelain mortar ^[5]		
<i>N</i> [%]	16.24		
Ω(CO ₂) [%]	−35.3		
<i>T</i> _{m,p.} [°C]	91–92 (crystals) ^[1] , 92 ^[2] , 91 (pure) ^[5] , 90.5 (crude) ^[5] , 79 ^[6]		
ρ [g cm ⁻³]	sp. gr. = 1.57 ^[1] , 1.61 ^[6]		
Heat of formation	144.3 kcal/mol ^[1]		
Heat of combustion	1,149.9 kcal/mol (@ C°) ^[1]		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
−Δ _{ex} <i>U</i> ^o [kJ kg ⁻¹]		1,035 kcal/kg ^[2] 4,330.44 ^[6]	1,035 kcal/kg ^[1]
<i>T</i> _{ex} [K]			

p_{C-J} [kbar]			
VoD [m s ⁻¹]		7,360 (@ 1.57 g cm ⁻³) ^[2]	5,060 (@ 0.75 g cm ⁻³) ^[1] 7,360 (@ 1.57 g cm ⁻³) ^[1] 24,200 ft/s (@ 1.5 g/mL) ^[3]
V_0 [L kg ⁻¹]			
Trauzl test [cm ³ , % TNT]	160% ^[1] , 480 cm ³ ^[4]		
Ballistic mortar test	15% TNT ^[1] , 1.51 × power of TNT (loose sample) ^[5]		
Vacuum stability test [cm ³ /h]	@ 80 °C: <0.5 mL after 60 min (5 g sample) ^[5] @ 95 °C: 11–13 mL in 24 h (acetone precipitated sample) ^[5] @ 95 °C: >14 mL in 24 h (EtOH cryst. sample) ^[5] @ 100 °C: 12–15 mL in 12 h (no difference between precipitated or recryst. samples) ^[5]		
Abel test	15–35 min @ 100 °C ^[5]		
Solubility [g/mL]	Soluble in acetone ^[5] , recryst. from EtOH, boiling benzene ^[5] , insoluble in water ^[6] , soluble in most organic solvents ^[6]		

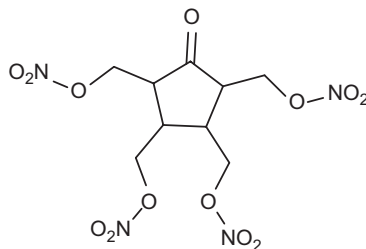
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Tetramethylolcyclopentanone tetranitrate

Name [German, acronym]: 2,2,5,5-Tetramethylolcyclopentanone tetranitrate
[nitropentanon, FIVONITE, FV]

Main (potential) use: Good plasticizer for NC, is suitable for use in some explosive and propellant mixtures

Structural formula:



	FIVONITE
Formula	$C_9H_{12}N_4O_{13}$
Molecular mass [$g\ mol^{-1}$]	384.21
Appearance at RT	White crystalline solid ^[9]
IS [J]	$H_{50\%} = 90\ cm$ (Bruceton no. 3 apparatus, 5 kg mass) ^[4] , 62% PA or similar to TNT ^[5] , $>90\ cm$ (ERL #3, sample in brass cup 0.308 in inside diameter, 0.01 in thick, $\frac{7}{8}$ in height, 5 kg mass) ^[11] , 38 cm (ERL #5, sample in cylindrical cavity $\frac{1}{16}$ in deep, 0.376 in inside diameter, 5 kg mass) ^[11] , 69 cm (ERL #12, sample on square of Flint paper, $2\frac{1}{2}$ kg mass) ^[11]
N [%]	14.58
$\Omega(CO_2)$ [%]	-45.8
$T_{m.p.}$ [°C]	$74^{[3, 4]}, 68-70^{[4]}, 68^{[9, 11]}$
$T_{dec.}$ [°C]	(Deflagration temp. = $265\ ^\circ C$) ^[4]
ρ [$g\ cm^{-3}$]	$1.59^{[3]}, 1.611$ (crystals @ $20\ ^\circ C$) ^[4] , 1.56 (@ $293\ K$) ^[1] , 1.590 (cast @ $20\ ^\circ C$) ^[4] , 1.499 (liq. @ freezing point) ^[4] , 1.59 (c) ^[11]
Heat of formation	$-1,760\ kJ/kg$ (enthalpy of form.) ^[3] , $166.3\ kcal/mol$ ^[4] , $172.57\ kcal/mol$ ($-\Delta H_f$, heat of form. @ standard conditions) ^[12]

Heat of combustion	1,093.5 kcal/mol ^[4] Exptl. heat of combustion data ^[12] : <table><tr><td>$-\Delta U_{B/M}$ (cal/g)</td><td>$-\Delta U_B$ (kcal/mol)</td><td>$-\Delta U_R$ (kcal/mol @ 1 atm. and constant vol.)</td><td>$-\Delta H_R$ (kcal/mol @ 1 atm. and constant pressure)</td></tr><tr><td>2,843.99 ± 1.43</td><td>1,092.71</td><td>1,090.85</td><td>1,097.60</td></tr></table>			$-\Delta U_{B/M}$ (cal/g)	$-\Delta U_B$ (kcal/mol)	$-\Delta U_R$ (kcal/mol @ 1 atm. and constant vol.)	$-\Delta H_R$ (kcal/mol @ 1 atm. and constant pressure)	2,843.99 ± 1.43	1,092.71	1,090.85	1,097.60
$-\Delta U_{B/M}$ (cal/g)	$-\Delta U_B$ (kcal/mol)	$-\Delta U_R$ (kcal/mol @ 1 atm. and constant vol.)	$-\Delta H_R$ (kcal/mol @ 1 atm. and constant pressure)								
2,843.99 ± 1.43	1,092.71	1,090.85	1,097.60								
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.								
$-\Delta_{ex}U^o$ [kJ kg ⁻¹]	4,719		820 kcal/kg ^[4]								
T_{ex} [K]	3,307										
p_{C-J} [kbar]	203										
VoD [m s ⁻¹]	7,158 (@ 1.55 g cm ⁻³)	6,780 (@ TMD, calcd., R-P method) ^[7]	7,040 (@ 1.59 g cm ⁻³) ^[2] 7,040 (@ 1.55 g cm ⁻³) ^[3] 7,292 (@ 1.57 g cm ⁻³) ^[4] 6,815 (@ 1.44 g cm ⁻³) ^[4] 7,300 (@ 1.57 g cm ⁻³) ^[6] 23,900 ft/s (@ 1.5 g/ml) ^[9] 7,160 (@ 1.57 g cm ⁻³) ^[11]								
V_0 [L kg ⁻¹]	747										

Trauzl test [cm ³ , % TNT]	129% TNT ^[4, 6] , 117% PA ^[5] , 387 cm ³ ^[10]
Ballistic mortar test	121–122% TNT ^[6] , 127% TNT ^[4] , 122% TNT ^[5] , 121% TNT ^[11]
5 s explosion T [°C] Explosion T [°C]	285 (Wood's metal surface) ^[4] T (°C)/time to explosion (s) ^[5] : 350/0.300, 320/0.490, 300/0.760, 232/3.35 ^[5]

	T (°C) and explosion time (s), 25 mg sample ^[8] :			
	T (°C)	Time (s)	T (°C)	Time (s)
	350	0.300	249	2.40
	320	0.490	232	3.35
	300	0.760	225	No explosion
	270	1.35		
	265 (deflagrates) ^[9] , no explosion <360 ^[9]			
Vacuum stability test [cm ³ /h]	5–10 cc gas evolved from 5 g sample in 48 h @ 100 °C ^[4]			
Bullet sensitivity	42 (l. l. (ord)) ^[11] , 58 (no l. l. (alz)) ^[11]			

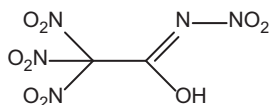
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Tetranitroacetimidic acid

Name [German, acronym]: Tetranitroacetimidic acid [TNAA]

Main (potential) use: Possible future oxidizer and replacement for AP^[1], proposed as an environmentally benign oxidizer^[2]

Structural formula:



	TNAA																													
Formula	C ₂ HN ₅ O ₉																													
Molecular mass [g mol ⁻¹]	239.06																													
Appearance at RT	Colorless crystals which turn slightly yellow over time ^[1]																													
IS [J]	19 ^[1]																													
FS [N]	<p>20^[1], triangular crystals obtained from dichloromethane sensitive to friction^[2] very thin, flake style particles obtained by precipitating from hexane showed less sensitivity^[2], 98 (crystalline TNAA from dichloromethane, average particle size = 112.4 μm)^[2]</p> <p>Concentrated TNAA soln. in dichloromethane (130 g/L) precipitated in 4 volume parts on the following liquids under constant stirring (Julius Peters apparatus)^[2]:</p> <table><tr><td>Liquid</td><td>Yield (%)</td><td>Particle size (μm)</td><td>Surface area (m² g⁻¹)</td><td>FS (N)</td></tr><tr><td>Pentane</td><td>90</td><td>2.07</td><td>1.55</td><td>118</td></tr><tr><td>Hexane</td><td>95</td><td>2.14</td><td>1.50</td><td>196</td></tr><tr><td>Cyclohexane</td><td>85</td><td>2.97</td><td>1.08</td><td>157</td></tr><tr><td>Heptane</td><td>75</td><td>2.03</td><td>1.58</td><td>137</td></tr></table>					Liquid	Yield (%)	Particle size (μm)	Surface area (m ² g ⁻¹)	FS (N)	Pentane	90	2.07	1.55	118	Hexane	95	2.14	1.50	196	Cyclohexane	85	2.97	1.08	157	Heptane	75	2.03	1.58	137
Liquid	Yield (%)	Particle size (μm)	Surface area (m ² g ⁻¹)	FS (N)																										
Pentane	90	2.07	1.55	118																										
Hexane	95	2.14	1.50	196																										
Cyclohexane	85	2.97	1.08	157																										
Heptane	75	2.03	1.58	137																										
N [%]	29.30																													
Ω(CO ₂) [%]	30.12																													
T _{m.p.} [°C]	91 ^[1] , 149.1 (TGA) ^[2]																													
T _{dec.} [°C]	137 (onset) ^[1] , 100 (onset), 160 (complete dec.) (TGA) ^[2]																													
ρ [g cm ⁻³]	1.87 (measured) ^[1] , 1.84 (crystal) ^[1]																													
Heat of formation	−134.6 kJ/mol (ΔH _f , calcd.) ^[1] , −0.563 kJ/g (ΔH _f , calcd.) ^[1]																													

	Calcd. (EXPLO5 6.01)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^\circ$ [kJ kg ⁻¹]			
T_{ex} [K]			
$p_{\text{C-J}}$ [kbar]	23 GPa (@ 1.84 g cm ⁻³ , $\Delta H_f = -134.7$ kJ/mol) ^[1]		
VoD [m s ⁻¹]	7,503 (@ 1.84 g cm ⁻³ , $\Delta H_f = -134.7$ kJ/mol) ^[1]		
V_0 [L kg ⁻¹]			
Thermal stability	Stable @ RT for long periods of time ^[1]		
Solubility [g/mL]	Only slightly soluble in most organic solvents ^[1] , partially soluble in ethyl acetate and dichloromethane ^[1] , unstable in acetonitrile ^[1] , can be recryst. from dichloromethane ^[1] , decomposition in DMSO and NMP ^[2] , hexane can be used as antisolvent ^[2]		
Hygroscopicity	Nonhygroscopic ^[1] , hydrolyzed by water ^[2]		
Compatibility	Unstable in acetonitrile (dec.) ^[1] , dec. in DMSO ^[1] , dec. in aqueous KOH, sodium bicarbonate, ammonia or guanidinium carbonate soln. ^[1] , decomposition in DMSO and NMP ^[2] , hydrolyzed by water ^[2] , inert toward HTPB and TDI (toluene diisocyanate) (FT-IR) ^[2]		
I_{sp} [s]	209 (calcd. EXPLO 5 6.01, @ isobaric pressure of 70 bar and initial T of 3,300 K) ^[1]		

	TNAA^[1]
Chemical formula	C ₂ H ₁ N ₅ O ₉
Molecular weight [g mol ⁻¹]	239.06
Crystal system	Monoclinic
Space group	$P2_1/c$
a [Å]	11.866(4)
b [Å]	6.713(2)
c [Å]	10.848(4)
α [°]	90
β [°]	93.929(4)
γ [°]	90

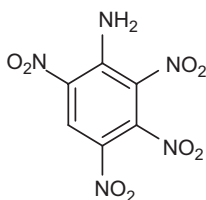
$V [\text{\AA}^3]$	862.0(5)
Z	4
$\rho_{\text{calc}} [\text{g cm}^{-3}]$	1.842
$T [\text{K}]$	293

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2,3,4,6-Tetranitroaniline

Name [German, acronym]: 2,3,4,6-Tetranitroaniline [tetranitroanilin, TNA, TeNA]
 Main (potential) use: Filler in bombs, mines, component of HE compositions, substitute for tetryl in detonators^[8], no practical use as a consequence of its low stability^[13], acts as a starting material for the preparation of other energetic materials^[13], too reactive to be suitable for application^[14], was used during World War I^[14], was used as an ingredient of cheap, relatively insensitive blasting explosives^[22], MF replacement in commercial blasting caps or electric detonators^[22], as a booster charge in ammunition^[22]

Structural formula:



	TNA
Formula	$C_6H_3N_5O_8$
Molecular mass [g mol ⁻¹]	273.12
Appearance at RT	Yellow crystals ^[13, 24] , yellowish-brown or greenish-brown crystals ^[13] , brownish crystals ^[21] , greenish-yellow to olive-green crystalline solid ^[22]
IS [J]	6 Nm ^[7] , log $H_{50\%} = 1.61$ ^[6] , FI = 86% of PA ^[8] , 54–55 cm (2 kg hammer, Kast apparatus) ^[8] , $H_{50\%} = 41$ cm ^[9, 12] , $H_{50\%} = 141$ cm (B.M., type 12 tool, 2.5 kg mass, 35 mg sample, garnet paper) ^[11] , same sensitivity as Tetryl ^[14] , 41 cm (2.5 kg mass) ^[16] , 27.7 cm (2.5 kg mass, AFATL) ^[16] , $H_{50} = 47$ cm (2.5 kg mass, type 12 tool) ^[17] , log(H_{50}) = 1.613 (<i>Kamlet/Adolph</i>) ^[18] , $H_{50\%} = 47$ cm (2.5 kg mass) ^[25]
N [%]	25.64
Ω(CO ₂) [%]	−32.2
$T_{m.p.}$ [°C]	207–211 ^[1] , 216 ^[7] , 216–217 (dec.) ^[8] , 215 (dec.) ^[13, 19] , 210 (melts with dec) ^[14, 21] , 210–215 (dec.) ^[22] , 217–220 (dec.) ^[24]
$T_{dec.}$ [°C]	220–230, 222 (puffs) ^[8] , 210 (melts with dec.) ^[14]
ρ [g cm ⁻³]	1.87 (@ 293 K) ^[2] , 1.867 ^[7] , 1.867 (crystal) ^[8] , sp. gr. = 1.867 ^[13, 24] , 1.861 ^[12]

Heat of formation	-179 kJ/kg (enthalpy of form.) ^[7] , 14.0 kcal/mol (Q_f) ^[8] , 25.4 kcal/kg ^[23] , -11.74 kcal/mol ($\Delta H_f(s)$) ^[12] , -48.9 kJ/mol (enthalpy of form., exptl.) ^[24] , -61.5 kJ/mol (enthalpy of form., calcd., emp.) ^[24] , -63.9 kJ/mol (enthalpy of form., calcd., S-D method) ^[24]		
Heat of combustion	654.3 kcal/mol (Q_c^V) ^[8] , 653 kcal/mol (Q_c^P) ^[8] , 2,411 kcal/kg (@ C^V) ^[23]		
	Calcd. (EXPLO5 5.04)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^0$ [kJ kg ⁻¹]	5,203	1.39 kcal/g (Q_{max} , calcd.) ^[12]	4,378 [H ₂ O (l)] ^[3, 7] 4,100 [H ₂ O (g)] ^[5] 4,280 [H ₂ O (g)] ^[7] 265.1 kcal/mol ^[8]
T_{ex} [K]	3,794	3,238 °C (calcd.) ^[8] 3,500 °C (calcd.) ^[8]	
p_{C-J} [kbar]	30.8	307 (@ 1.861 g cm ⁻³ , calcd.) ^[12]	
VoD [m s ⁻¹]	8,375 (@ TMD)	8,240 (@ 1.861 g cm ⁻³ , calcd.) ^[12]	7,300 (@ 1.5 g cm ⁻³) ^[5] 7,630 (@ 1.6 g cm ⁻³) ^[8] 25,000 ft/s (@ 1.6 g/mL) ^[19] 7,500 (@ 1.6 g cm ⁻³) ^[21]
V_0 [L kg ⁻¹]	657		813 ^[4, 7] 10.55 L gas produced on explosion of 1 g TNA @ 3,238 °C ^[8]

Trauzl test [cm ³ , % TNT]	130–149% TNT ^[10] , 140% TNT (average value) ^[8] , 430 cc (10 g sample, cf. 254 cc for TNT, 297 cc for PA) ^[14] , 430 cc (i.e., 10–15% higher than for Tetryl) ^[24]
Sand test [g]	102% TNT ^[8, 10] , 56.3 g (amount of sand crushed finer than 30 mesh, by total charge consisting of base charge of 0.50 g tetranitroaniline and 0.30 g priming charge of MF) ^[20] , 44.6 g (amount of sand crushed finer than 30 mesh, by base charge of 0.50 g tetranitroaniline) ^[20] , rel. strength cf. TNT = 1.02 ^[20]

Ballistic mortar test	121% TNT ^[10] , 121% TNT (average value) ^[8]
Initiation efficiency	<p>Minimum initiating charge of primary explosive (g) required to initiate 0.4 g TNA (0.4 g TNA in detonator capsule, pressed down, initiator added on top, covered with reinforcing cap, pressed @ 200 atm./in²)^[15]: 0.09 g cyanuric azide^[15], 0.20 g mercury fulminate^[15]</p> <p>Minimum initiating charge of primary explosive (g) required to initiate 0.5 g TNA (0.5 g TNA in No. 8 detonator shell, primary explosive added on top, both compressed under reinforcing capsule @ 3,400 lb/in²)^[15]: 0.085 g DDNP^[15], 0.175 g mercury fulminate^[15], 0.05 g LA^[15]</p> <p>Minimum initiating charge of primary explosive (g) required to initiate 0.4 g TNA (0.5 g TNA compressed in detonator capsules @ 1,000 lb/in²)^[15]: 0.20 g fulminate with reinforcing cap^[15], 0.05 g HMTD with reinforcing cap^[15], 0.05 g HMTD without reinforcing cap^[15]</p>
5 s explosion <i>T</i> [°C] Explosion <i>T</i> [°C] Initiation <i>T</i> [°C]	237 (@ 5 °C/min) ^[8] , 247 (@ 20 °C/min) ^[8] , ~ 237 ^[19] 231–233 ^[13] , 226 (deflagrates) ^[14, 21]
Thermal stability	Heat test: dec. @ 65.5 °C if traces of moisture are present ^[13] , long storage stability not very satisfactory particularly in the presence of moisture ^[21] , completely stable in dry storage ^[22] , long-term exposure to moisture promotes hydrolysis ^[22] , storage for 9 years during World War I showed significant deterioration ^[24]
Vacuum stability test [cm ³ /h]	Industrial sample: 0.34 cc/g/h in first 16 h @ 100 °C, 0.020 cc/g/h in 17–32 h period, 0.015 cc/g/h in 33–48 h period ^[8] sample stored for ~ 10 months: 1.39 cc/g gas evolved in 30 h @ 120 °C ^[8]
Solubility [g/mL]	Poorly soluble in common organic solvents ^[13, 24] , soluble in acetone and <i>o</i> -nitrotoluene ^[13] , readily soluble in acetone (1 part in 6 parts acetone @ boiling temp.) ^[14] , readily soluble in glacial acetic acid (1 part in 24 parts glacial acetic acid @ boiling temp.) ^[14] , sparingly soluble in benzene and CHCl ₃ ^[14] , insoluble in water ^[24] , can be recryst. from nitroxylenes ^[24]
Hygroscopicity	Moisture on long-term storage promotes hydrolysis ^[21] , nonhygroscopic ^[22] , virtually nonhygroscopic ^[24]
Compatibility	Does not attack metals ^[19, 22] , moisture on long-term storage promotes hydrolysis ^[21] , no reaction with water @ RT but vigorous reaction @ 50 °C ^[24] , reacts with aqueous sodium acetate @ RT ^[24]
Dipole moment [D]	4.85 (calcd.) ^[16]
Rifle bullet test	Readily detonated by rifle bullet ^[22]
Abel test	Withstands @ 71 °C for 1 h ^[24]
Flash point [°C]	222–223 ^[24]

	TNA^[2]
Chemical formula	C ₆ H ₃ N ₅ O ₈
Molecular weight [g mol ⁻¹]	273.12
Crystal system	Monoclinic
Space group	<i>P</i> 2 ₁ / <i>c</i> (no. 14)
<i>a</i> [Å]	7.270(10)
<i>b</i> [Å]	11.060(20)
<i>c</i> [Å]	12.270(20)
α [°]	90
β [°]	98.80(30)
γ [°]	90
<i>V</i> [Å ³]	974.97
<i>Z</i>	4
ρ_{calc} [g cm ⁻³]	1.861
<i>T</i> [K]	295

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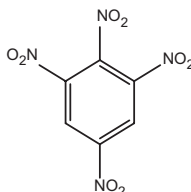
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Tetranitrobenzene

Name [German, acronym]: 1,2,3,5-Tetranitrobenzene, 1,2,4,6-tetranitrobenzene
[tetranitrobenzol, TetNB, TETNB]

Main (potential) use: high explosive

Structural formula:



	Tetranitrobenzene
Formula	$C_6H_2N_4O_8$
Molecular mass [g mol ⁻¹]	258.10
Appearance at RT	Bright yellow crystalline solid (1,2,3,5-isomer) ^[1] , fine yellow needles ^[5] , yellow solid (1,2,3,4-isomer) ^[11]
IS [J]	$H_{50\%} = 28$ cm (log h = 1.45, type 12 tool, 2.5 kg mass, 35 mg sample, garnet paper, B.M.) ^[3] , $H_{50} = 0.27$ m (cf. 4.90 m for TATB) ^[8] , $H_{50} = 33$ cm ^[9] , $H_{50\%} = 28$ cm (2.5 kg mass) ^[12]
N [%]	21.71
$\Omega(CO_2)$ [%]	-31.00
$T_{m.p.}$ [°C]	129–130 (1,2,3,5-isomer) ^[1, 11] , 116 (crystals) ^[5] , 124–125 (recryst.) ^[6] , 125–129 (recryst.) ^[6] , 108–109 (1,2,3,4-isomer) ^[11] , 127–129 (no isomer specified) ^[11]
$T_{dec.}$ [°C]	
ρ [g cm ⁻³]	1.82 ^[3]
Heat of formation	-30.9 kcal/mol (ΔH_f (g) @ 25 °C, 1,2,3,4-isomer, calcd., MINDO/3) ^[10] , -31.6 kcal/mol (ΔH_f (g) @ 25 °C, 1,2,3,5-isomer, calcd., MINDO/3) ^[10] , -32.0 kcal/mol (ΔH_f (g) @ 25 °C, 1,2,4,5-isomer, calcd., MINDO/3) ^[10] , 112.5 kcal/mol (ΔH_f (g) @ 25 °C, 1,2,3,4-isomer, calcd., MNDO) ^[10] , 110.1 kcal/mol (ΔH_f (g) @ 25 °C, 1,2,3,5-isomer, calcd., MNDO) ^[10] , 109.9 kcal/mol (ΔH_f (g) @ 25 °C, 1,2,4,5-isomer, calcd., MNDO) ^[10]

	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^\circ$ [kJ kg ⁻¹]			
T_{ex} [K]			
$p_{\text{C-J}}$ [kbar]		33.38 GPa (@ 1.90 g cm ⁻³ , calcd., K-J) ^[4]	
VoD [m s ⁻¹]		8,530 (@ 1.90 g cm ⁻³ , calcd., K-J) ^[4]	
V_0 [L kg ⁻¹]			
Thermal stability	Virtually no dec. on storage in air ^[1]		
Solubility [g/mL]	1,2,3,5-isomer soluble in EtOH, acetone, Et ₂ O ^[1] , some solubility in hydrocarbons and halocarbons ^[1] , practically insoluble in H ₂ O ^[1] , easily soluble in EtOH, Et ₂ O, glacial acetic acid ^[5] , recryst. from CCl ₄ (1,2,3,4-isomer) ^[11]		
Compatibility	1,2,3,5-isomer slowly reacts with H ₂ O turning soln. yellowish ^[1] , rapid conversion of 1,2,3,5-isomer to PA in boiling H ₂ O ^[1] , forms red complexes in presence of hydroxide or sulfide ion in water or ethoxide ion in ethanol ^[7]		

	1,2,4,6-Tetranitrobenzene ^[2]
Chemical formula	C ₆ H ₂ N ₄ O ₈
Molecular weight [g mol ⁻¹]	
Crystal system	Orthorhombic
Space group	<i>P</i> 2 ₁ 2 ₁ 2 ₁ (no. 19)
<i>a</i> [Å]	12.4
<i>b</i> [Å]	13.1
<i>c</i> [Å]	6.15
α [°]	90
β [°]	90
γ [°]	90
<i>V</i> [Å ³]	999.006
<i>Z</i>	4
ρ_{calc} [g cm ⁻³]	1.716
<i>T</i> [K]	295

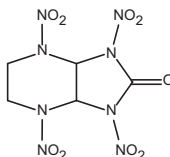
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Tetranitro-bicyclo-nonanone

Name [German, acronym]: 1,3,4,7-Tetranitrooctahydro-2*H*-imidazo[4,5-*b*]pyrazin-2-one [K56]

Main (potential) use: under research

Structural formula:



	K56		
Formula	C ₅ H ₆ N ₈ O ₉		
Molecular mass [g mol ⁻¹]	322.15		
Appearance at RT			
IS [J]			
FS [N]			
ESD [J]			
<i>N</i> [%]	34.78		
Ω(CO ₂) [%]	-19.87		
<i>T</i> _{m.p.} [°C]			
<i>T</i> _{dec.} [°C]			
<i>ρ</i> [g cm ⁻³]	1.975 ^[1]		
Heat of formation	-144 kJ/mol (enthalpy of form.) ^[1]		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
-Δ _{ex} <i>U</i> ^o [kJ kg ⁻¹]			
<i>T</i> _{ex} [K]			
<i>p</i> _{C-J} [kbar]			
VoD [m s ⁻¹]			
<i>V</i> ₀ [L kg ⁻¹]			

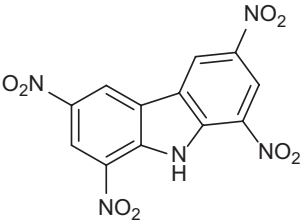
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Tetranitrocarbazole

Name [German, acronym]: Tetranitrocarbazole, 1,3,6,8-tetranitrocarbazole, tetranitrodibenzopyrrole, nitrosan [tetranitrocarbazol, TNC, TeNCbz]

Main (potential) use: Ingredient in pyrotechnic compositions, igniter^[3], energetic fuel in some propellants^[10], some pyrotechnic compositions^[10]

Structural formula:



	TNC
Formula	C ₁₂ H ₅ N ₅ O ₈
Molecular mass [g mol ⁻¹]	347.20
Appearance at RT	Light yellow solid ^[3] , yellow crystals ^[10]
IS [J]	19.62 (100 + cm, 2 kg mass, 20 mg sample, B.M.) ^[3] , 18 in (14 mg sample, 2 kg mass, P.A.) ^[3, 6] , 28 in (2 kg mass, confined, height of no detonation, P.A.) ^[10]
FS [N]	Unaffected by steel shoe (friction pendulum test) ^[3] , unaffected by fiber shoe (friction pendulum test) ^[3]
N [%]	20.17
Ω(CO ₂) [%]	−85.3
T _{m.p.} [°C]	296 ^[1, 4, 5, 9] , 296 (for pure 1,3,6,8-isomer) ^[3] , 280 for crude product ^[3] , 300 ^[10]
T _{dec.} [°C]	Yellow crystals turn red-brown above 200 °C ^[10]
ρ [g cm ⁻³]	1.893 (@ 293 K) ^[2] , 1.765 (@ 173 K) ^[4] , 1.73 (@ 20 °C, pycnometer) ^[4]
Heat of formation	54.4 kJ/kg (enthalpy of form.) ^[5] , −18.9 kJ/mol ^[4] , −6.9 kcal/mol (Q _f) ^[6] , 28.3 kcal/kg (energy of form.) ^[7] , 13.0 kcal/kg (enthalpy of form.) ^[7] , −18.9 kJ/mol (enthalpy of form.) ^[10] , 18.9 kJ/mol (enthalpy of form., exptl.) ^[11] , 24.0 kJ/mol (enthalpy of form., calcd., emp.) ^[11] , 3.2 kJ/mol (enthalpy of form., calcd., S-D method) ^[11]
Heat of combustion	1,310 kcal/mol ^[6]

	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^\circ$ [kJ kg ⁻¹]	3,738	890 kcal/kg ^[7]	3,433 [H ₂ O (l)] ^[5]
T_{ex} [K]	2,812		
$p_{\text{C-J}}$ [kbar]	205		
VoD [m s ⁻¹]	7,125 (@ TMD)		
V_0 [L kg ⁻¹]	543		

Sand test [g]	41.3 g (200 g bomb) ^[3] , 86–95% TNT ^[6]																
Initiation efficiency	0.20 g LA minimum detonating charge ^[3] , 0.25 g Tetryl (minimum detonating charge) ^[3]																
5 s explosion T [°C] 5 s ignition T [°C]	470 ^[6] , 470 (dec.) ^[3] 470 (dec.) ^[8]																
100 °C heat test [% mass loss]	0.15% mass loss in first 48 h ^[3, 6] , 0.05% mass loss in second 48 h ^[3, 6] , no explosion in 100 h ^[3, 6]																
Thermal stability	Can be dried as thin layer @ 100–110 °C for 4 h ^[3]																
Vacuum stability test [cm ³ /h]	0.2 cc/40 h @ 100 °C ^[3] , 0.2 cc/40 h @ 120 °C ^[3]																
Solubility [g/mL]	0.10 g / 100 g H ₂ O @ 95 °C ^[3] , insoluble in water ^[10]																
Hygroscopicity	<p>0.01% @ 30 °C with 90% RH^[3], very soluble in nitrobenzene^[3], soluble in acetone^[3], insoluble in benzene, CHCl₃, CCl₄, Et₂O and petroleum ether^[3]</p> <p>Qualitative solubilities^[3]:</p> <table border="1"> <tr> <th>Solvent</th><th>Solubility</th></tr> <tr> <td>Nitrobenzene</td><td>Very soluble</td></tr> <tr> <td>Acetone</td><td>Soluble</td></tr> <tr> <td>Benzene</td><td>Insoluble</td></tr> <tr> <td>Chloroform</td><td>Insoluble</td></tr> <tr> <td>Carbon tetrachloride</td><td>Insoluble</td></tr> <tr> <td>Ether</td><td>Insoluble</td></tr> <tr> <td>Ether, petroleum</td><td>Insoluble</td></tr> </table>	Solvent	Solubility	Nitrobenzene	Very soluble	Acetone	Soluble	Benzene	Insoluble	Chloroform	Insoluble	Carbon tetrachloride	Insoluble	Ether	Insoluble	Ether, petroleum	Insoluble
Solvent	Solubility																
Nitrobenzene	Very soluble																
Acetone	Soluble																
Benzene	Insoluble																
Chloroform	Insoluble																
Carbon tetrachloride	Insoluble																
Ether	Insoluble																
Ether, petroleum	Insoluble																
Flash point [°C]	350 ^[10]																

	Tetranitrocarbazole ^[4]
Chemical formula	C ₁₂ H ₅ N ₅ O ₈
Molecular weight [g mol ⁻¹]	347.21
Crystal system	Monoclinic
Space group	<i>P</i> 2 ₁ / <i>c</i> (no. 14)
<i>a</i> [Å]	
<i>b</i> [Å]	
<i>c</i> [Å]	
α [°]	
β [°]	
γ [°]	
<i>V</i> [Å ³]	
<i>Z</i>	
ρ_{calc} [g cm ⁻³]	1.765
<i>T</i> [K]	−100 °C

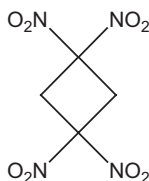
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1,1,3,3-Tetranitrocyclobutane

Name [German, acronym]: Tetranitrocyclobutane [TNCB]

Main (potential) use: high explosive

Structural formula:



	TNCB		
Formula	$C_4H_4N_4O_8$		
Molecular mass [g mol ⁻¹]	236.09		
Appearance at RT	Clear, colorless plate crystals ^[1]		
IS [J]			
FS [N]			
ESD [J]			
N [%]	23.73		
$\Omega(CO_2)$ [%]	-13.55		
$T_{m.p.}$ [°C]	165 ^[2]		
$T_{b.p.}$ [°C]			
$T_{phase\ transition}$ [°C]			
$T_{dec.}$ [°C]			
ρ [g cm ⁻³]	1.83 ^[2]		
Heat of formation	-84 kJ/mol		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{ex}U^\circ$ [kJ kg ⁻¹]	6178		
T_{ex} [K]	4222		

p_{C-1} [kbar]	339		
VoD [m s ⁻¹]	8646		
V_0 [L kg ⁻¹]	706		

	TNCB^[1]
Chemical formula	C ₄ H ₈ N ₄ O ₈
Molecular weight [g mol ⁻¹]	236.1
Crystal system	Triclinic
Space group	<i>P</i> -1
<i>a</i> [Å]	6.301 (1)
<i>b</i> [Å]	7.858 (1)
<i>c</i> [Å]	8.736 (1)
α [°]	85.88 (1)
β [°]	84.62 (1)
γ [°]	85.13 (1)
<i>V</i> [Å ³]	428.2 (1)
<i>Z</i>	2
ρ_{calc} [g cm ⁻³]	1.831
<i>T</i> [K]	295

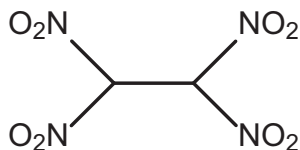
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Tetranitroethane

Name [German, acronym]: 1,1,2,2-Tetranitroethane [tetranitroethan, TNE]
 Main (potential) use: Possible precursor for high-performance energetic materials^[1]

Structural formula:



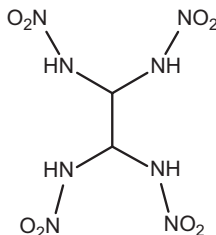
	TNE		
Formula	$\text{C}_2\text{H}_2\text{N}_4\text{O}_8$		
Molecular mass [g mol^{-1}]	210.06		
Appearance at RT			
N [%]	26.67		
$\Omega(\text{CO}_2)$ [%]	+22.9		
$T_{\text{m.p.}}$ [$^{\circ}\text{C}$]			
$T_{\text{dec.}}$ [$^{\circ}\text{C}$]			
ρ [g cm^{-3}]			
Heat of formation	−19.8 kcal/mol (ΔH_f (g) @ 25 $^{\circ}\text{C}$, calcd., MINDO/3) ^[2] , 86.1 kcal/mol (ΔH_f (g) @ 25 $^{\circ}\text{C}$, calcd., MNDO) ^[2]		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
− $\Delta_{\text{ex}}U^{\circ}$ [kJ kg^{-1}]			
T_{ex} [K]			
$p_{\text{C-J}}$ [kbar]			
VoD [m s^{-1}]			
V_0 [L kg^{-1}]			
Dipole moment, μ [D]	0.07 (calcd., MINDO/3, (g) @ 25 $^{\circ}\text{C}$) ^[2] , 0.02 (calcd., MNDO (g) @ 25 $^{\circ}\text{C}$) ^[2]		

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***N,N',N'',N'''*-Tetranitro-1,1,2,2-ethanetetramine**Name [German, acronym]: *N,N',N'',N'''*-Tetranitro-1,1,2,2-ethanetetramine [TNAE]Main (potential) use: Potential new energetic material^[1]

Structural formula:



	TNAE		
Formula	$C_2H_6N_8O_8$		
Molecular mass [g mol ⁻¹]	270.12		
Appearance at RT			
IS [J]	$H_{50} = 0.76$ kp-m (2 kg mass, @ 20 °C, ~ 45% RH, 25 tests, BAM) ^[1]		
FS [N]	8.3 kp (BAM) ^[1]		
<i>N</i> [%]	41.48		
$\Omega(CO_2)$ [%]	5.92		
$T_{m.p.}$ [°C]			
$T_{dec.}$ [°C]	143 (onset), 145 (peak max.) (DSC, @ 10 °C/min, N ₂ flow = 50 mL/min, Al cup with pierced lid) ^[1] 415.0 K (T_p , DSC @ 5 K/min) ^[2] , 421.1 K (T_p , DSC @ 10 K/min) ^[2] , 425.0 K (T_p , DSC @ 15 K/min) ^[2] , 427.9 K (T_p , DSC @ 20 K/min) ^[2] , 430.0 K (T_p , DSC @ 25 K/min) ^[2]		
ρ [g cm ⁻³]	1.87 ^[1] , 1.89 (He pycnometer) ^[1]		
Heat of formation	40.9 kcal/mol ($\Delta_f H^\circ$ (g), calcd.) ^[1] , 11.6 kcal/mol ($\Delta_f H^\circ$ (s), calcd.) ^[1] , 12.5 kcal/mol (calcd.) ^[1]		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{ex}U^\circ$ [kJ kg ⁻¹]		1,373.80 cal/g (calcd.) ^[1]	

T_{ex} [K]			
p_{CJ} [kbar]		39.25 GPa (calcd.) ^[1] 37.6 GPa (@ 1.89 g cm ⁻³ , calcd., BKWC, $\Delta_f H^\circ$ (s) = 12.5 kcal/mol) ^[1]	
VoD [m s ⁻¹]		8,760 (@ 1.87 g cm ⁻³ , calcd.) ^[1] 9,580 (@ 1.89 g cm ⁻³ , calcd., BKWC, $\Delta_f H^\circ$ (s) = 12.5 kcal/mol) ^[1]	
V_0 [L kg ⁻¹]			
ΔH_{sub} [kcal/mol]	29.3 ^[1]		

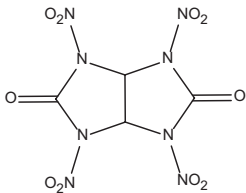
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Tetranitroglycolurile

Name [German, acronym]: Tetranitroglycolurile, tetranitroacetylenediurein, 2,4,6,8-tetranitro-2,4,6,8-tetraazabicyclo[3.3.0]octane-3,7-dione [Sorguyl, TNGU]

Main (potential) use: Highly explosive^[1], first patented in 1975^[18], potential for use in self-remediating formulations that are specifically designed to have short lifetimes in the environment after deployment (reduction of UXO environmental hazards)^[18]

Structural formula:



	Sorguyl	
Formula	C ₄ H ₂ N ₈ O ₁₀	
Molecular mass [g mol ⁻¹]	322.11	
Appearance at RT	Small clumps of fine needle crystals ^[18] , spherical morphology also obtained ^[18]	
IS [J]	2.04 ^[1] , <i>H</i> ₅₀ = 10.4 cm ^[1] , 0.15–0.2 ((no units) based on TNT = 1) ^[5] , 0.15–0.2 kg m ^[8] , 2 in (2 kg mass, P.A.) ^[8] , 6 cm (2 kg mass, B.M.) ^[8] , <i>A</i> _{d1} = 100% ^[16] , <i>H</i> _{50%} = 4.09 in ^[18]	
	IS data of various morphologies of TNGU, <i>H</i> ₅₀ , 5 lb mass, Lanlie one-shot method ^[18] :	
	Morphology	Impact (in)
	Sample prepared by lit. method	4.09
	TNGU prepared from imidazo imidazoles	11.06
	Sample prepared by lit. method, sphericalized	13.07
	TNGU prepared from nitrate salt, sphericalized	15.39

	<p>IS data of various morphologies of TNGU, H_{50}, 2 kg mass, Lanlie one-shot method^[18]:</p> <table> <tr> <th>Morphology</th><th>Impact (cm)</th></tr> <tr> <td>Sample prepared by lit. method</td><td>10.4</td></tr> <tr> <td>TNGU prepared from imidazo imidazoles</td><td>28.1</td></tr> <tr> <td>Sample prepared by lit. method, sphericalized</td><td>33.2</td></tr> <tr> <td>TNGU prepared from nitrate salt, sphericalized</td><td>29.1</td></tr> </table>	Morphology	Impact (cm)	Sample prepared by lit. method	10.4	TNGU prepared from imidazo imidazoles	28.1	Sample prepared by lit. method, sphericalized	33.2	TNGU prepared from nitrate salt, sphericalized	29.1
Morphology	Impact (cm)										
Sample prepared by lit. method	10.4										
TNGU prepared from imidazo imidazoles	28.1										
Sample prepared by lit. method, sphericalized	33.2										
TNGU prepared from nitrate salt, sphericalized	29.1										
FS [N]	<p>54^[1, 18]</p> <p>FS data of various morphologies of TNGU, H_{50}, Julius-Peters, BAM^[1, 18]:</p> <table> <tr> <th>Morphology</th><th>Friction (N)</th></tr> <tr> <td>Sample prepared by lit. method</td><td>54</td></tr> <tr> <td>TNGU prepared from imidazo imidazoles</td><td>70</td></tr> <tr> <td>Sample prepared by lit. method, sphericalized</td><td>72</td></tr> <tr> <td>TNGU prepared from nitrate salt, sphericalized</td><td>94</td></tr> </table>	Morphology	Friction (N)	Sample prepared by lit. method	54	TNGU prepared from imidazo imidazoles	70	Sample prepared by lit. method, sphericalized	72	TNGU prepared from nitrate salt, sphericalized	94
Morphology	Friction (N)										
Sample prepared by lit. method	54										
TNGU prepared from imidazo imidazoles	70										
Sample prepared by lit. method, sphericalized	72										
TNGU prepared from nitrate salt, sphericalized	94										
ESD [J]	<p>3.25^[1]</p> <p>ESD data of various morphologies of TNGU, ABL Laboratories ESD apparatus^[1, 18]:</p> <table> <tr> <th>Morphology</th><th>ESD (J)</th></tr> <tr> <td>Sample prepared by lit. method</td><td>3.25</td></tr> <tr> <td>TNGU prepared from imidazo imidazoles</td><td>3.25</td></tr> <tr> <td>Sample prepared by lit. method, sphericalized</td><td>3.25</td></tr> <tr> <td>TNGU prepared from nitrate salt, sphericalized</td><td>3.25</td></tr> </table>	Morphology	ESD (J)	Sample prepared by lit. method	3.25	TNGU prepared from imidazo imidazoles	3.25	Sample prepared by lit. method, sphericalized	3.25	TNGU prepared from nitrate salt, sphericalized	3.25
Morphology	ESD (J)										
Sample prepared by lit. method	3.25										
TNGU prepared from imidazo imidazoles	3.25										
Sample prepared by lit. method, sphericalized	3.25										
TNGU prepared from nitrate salt, sphericalized	3.25										
N [%]	34.79										
$\Omega(\text{CO}_2)$ [%]	5.0										
$T_{\text{m.p.}}$ [°C]	241 ^[2] , 190 ^[5]										
$T_{\text{dec.}}$ [°C]	237 (deflagration) ^[9] , 217–220 (DSC @ 10 °C/min) ^[1, 18]										
ρ [g cm ⁻³]	2.51 ± 0.1 (@ 293.15 K) ^[3] , 2.03–2.04 ^[5] , 2.01 ^[10, 13] , 2.04 ^[13] , 2.04 (@ TMD) ^[14] , 2.01 (measured) ^[18] , 2.01 (CHEETAH database) ^[1]										
Heat of formation	41.8 kJ/mol ($\Delta_f H^\circ$, EXPLO5 6.04), 379.0 kcal/kg ($\Delta_f H^\circ$) ^[7] , –33.5 kJ/mol (ΔH_f°) ^[13] , 379.0 kcal/kg (enthalpy of form.) ^[12] , 50.21 kJ/mol ^[14] , 50 kJ/mol (ΔH_f) ^[18] , 50 kJ/mol (ΔH_f , CHEETAH 7.0 database) ^[1]										

	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^{\circ}$ [kJ kg ⁻¹]	5,745	11.78 kJ/mL (calcd. CHEETAH 7.0) ^[1] 1,218 kcal/kg (@ 1.510 g cm ⁻³ , calcd.) [H ₂ O vapor] ^[12]	1,200 kcal/kg [H ₂ O (g)] ^[7] 1,200 kcal/kg (@ 1.510 g cm ⁻³) [H ₂ O vapor] ^[12]
T_{ex} [K]	4,177	4,088 (@ 2.01 g cm ⁻³ , $\Delta H_f = 50$ kJ/mol, calcd., JAGUAR) ^[15]	
$p_{\text{C-J}}$ [GPa]	40.2	41.77 (calcd., CHEETAH 7.0) ^[1] 40.5 (@ 2.01 g cm ⁻³ , $\Delta H_f = 50$ kJ/mol, calcd., JAGUAR) ^[15] 38.7 GPa (@ 1.98–2.01 g cm ⁻³) ^[17]	
VoD [m s ⁻¹]	9,446 (@ 2.02 g cm ⁻³ ; $\Delta_f H = 41.8$ kJ mol ⁻¹)	9,566 (@ 2.01 g cm ⁻³ , calcd., CHEETAH 7.0) ^[1] 8,850 (@ 2.01 g cm ⁻³ (TMD), calcd., R-P method) ^[11] 9,460 (@ 2.01 g cm ⁻³ , $\Delta H_f = 50$ kJ/mol, calcd., JAGUAR) ^[15] 9,200 (@ 1.98–2.01 g cm ⁻³) ^[17]	9,070 (@ 1.94 g cm ⁻³) ^[4] 9,330 ^[5] 9,150 (@ 1.95 g cm ⁻³) ^[6]
V_0 [L kg ⁻¹]	718		

Summary of experimental copper cylinder wall velocity data, samples have a wall thickness/diameter ratio of 0.1, cylinders were 305 mm long, PETN with $\rho = 1.763$ g cm⁻³ is the reference explosive^[14]:

Initial density (g/cm ³)	Inner diameter (mm)	Wall thickness (mm)	Wall velocity (mm/μs) at 25.4 mm diameter for R-R ₀ equal to			Velocity-squared cf. with PETN for the same configuration, % comparison R-R ₀ equal to		
			6 mm	12.5 mm	19 mm	6 mm	12.5 mm	19 mm
1.885	25.42	2.598	1.600	1.750	1.825	5.2	5.3	3.9

Summary of code calculations with measured detonation velocities and detonation energies derived from JWL's^[14]:

Initial density (g/cm ³)	PETN-adjusted BKWR Tiger, LLNL library $\theta = 1,850$ K, at v			JCZ3, LLNL library, v			CHEQ V2.4, at v		
	2.2	4.1	6.5	2.2	4.1	6.5	2.2	4.1	6.5
1.885	-2	-2	-1	-1	-4	-3	-9	-9	-8

Sand test [g]	61.9 g sand crushed (cf. 48.0 g for TNT) ^[8]														
5 s explosion T [°C] Explosion T [°C]	133 ^[8]														
100 °C heat test [% mass loss] 75 °C heat test [% mass loss]	Exploded in 30 min ^[8]														
Burn rate [mm/s]	Pressure interval = 0.6–15 MPa, pressure exponent = 0.867, burning rate @ 10 MPa = 44.4 mm/s, strand $\rho = 1.58 \text{ g cm}^{-3}$, adiabatic flame T @ 10 MPa = 3,395 K (measured using window constant pressure bomb) ^[13]														
Solubility [g/mL]	Soluble in 100% nitric acid ^[1, 18] , insoluble in CH_2Cl_2 ^[1, 18]														
Hygroscopicity	Decomposition in humid air (85% RH) according to $(t_{50} = 3.67 \text{ days})$ ^[17] : <table border="1"> <thead> <tr> <th>Time (days)</th><th>R_t (%)</th></tr> </thead> <tbody> <tr> <td>0</td><td>100</td></tr> <tr> <td>0.9375</td><td>97.449</td></tr> <tr> <td>1.583</td><td>92.720</td></tr> <tr> <td>2.354</td><td>85.496</td></tr> <tr> <td>3.3125</td><td>65.500</td></tr> <tr> <td>4.792</td><td>2.579</td></tr> </tbody> </table>	Time (days)	R_t (%)	0	100	0.9375	97.449	1.583	92.720	2.354	85.496	3.3125	65.500	4.792	2.579
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	<p>Decomposition in dry air (28% RH) according to ($t_{50} = 240 \pm 19$ days)^[17]:</p> <table border="1" data-bbox="444 232 740 582"> <thead> <tr> <th>Time (days)</th><th>R_t (%)</th></tr> </thead> <tbody> <tr><td>0</td><td>100</td></tr> <tr><td>5.854</td><td>97.553</td></tr> <tr><td>13.958</td><td>96.552</td></tr> <tr><td>33.815</td><td>98.068</td></tr> <tr><td>47.058</td><td>95.798</td></tr> <tr><td>60.961</td><td>96.829</td></tr> <tr><td>74.726</td><td>91.032</td></tr> <tr><td>125.797</td><td>87.254</td></tr> </tbody> </table> <p>Unstable in moist atmosphere and in presence of water^[18], half-life if exposed to atmosphere with relative humidity approaching 85% can be in the order of days^[18]</p>	Time (days)	R_t (%)	0	100	5.854	97.553	13.958	96.552	33.815	98.068	47.058	95.798	60.961	96.829	74.726	91.032	125.797	87.254																
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Compatibility	<p>Decomposition in humid air (85% RH) according to ($t_{50} = 3.67$ days)^[17]:</p> <table border="1" data-bbox="444 769 740 1042"> <thead> <tr> <th>Time (days)</th><th>R_t (%)</th></tr> </thead> <tbody> <tr><td>0</td><td>100</td></tr> <tr><td>0.9375</td><td>97.449</td></tr> <tr><td>1.583</td><td>92.720</td></tr> <tr><td>2.354</td><td>85.496</td></tr> <tr><td>3.3125</td><td>65.500</td></tr> <tr><td>4.792</td><td>2.579</td></tr> </tbody> </table> <p>99.6% dec. after 26 h in moist soil expt. with $t_{50} = \sim 1.72$ h^[17]</p> <p>Decomposition in dry soil (28% air RH) according to ($t_{50} = 202 \pm 35$ days)^[17]:</p> <table border="1" data-bbox="444 1190 740 1579"> <thead> <tr> <th>Time (days)</th><th>R_f (%)</th></tr> </thead> <tbody> <tr><td>0</td><td>100</td></tr> <tr><td>5.871</td><td>98.905</td></tr> <tr><td>12.020</td><td>100.142</td></tr> <tr><td>17.968</td><td>98.865</td></tr> <tr><td>33.840</td><td>93.059</td></tr> <tr><td>47.091</td><td>84.492</td></tr> <tr><td>60.990</td><td>87.256</td></tr> <tr><td>74.792</td><td>81.580</td></tr> <tr><td>125.822</td><td>79.292</td></tr> </tbody> </table> <p>Unstable in presence of water – even moist atmosphere^[18]</p>	Time (days)	R_t (%)	0	100	0.9375	97.449	1.583	92.720	2.354	85.496	3.3125	65.500	4.792	2.579	Time (days)	R_f (%)	0	100	5.871	98.905	12.020	100.142	17.968	98.865	33.840	93.059	47.091	84.492	60.990	87.256	74.792	81.580	125.822	79.292
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Many morphologies of TNGU have been reported^[1, 18], spherical morphology obtained using solvent/antisolvent method by dissolving TNGU in 100% nitric acid and precipitating it by addition beneath the surface of dichloromethane^[1, 18], small clumps of fine needle crystals usually obtained from literature procedures^[1, 18], TNGU derived from certain imidazo imidazoles obtained as thicker and longer needles^[1, 18], a summary of the methods for producing spherical TNGU morphologies is given below^[18]:

Scale (mg)	HNO ₃ (mL)	DCM (mL)	Stir rate (rpm)	Morphology
25	0.025	1	0	Cubes
25	0.025	10	0	Spheres and needles
25	0.025	10	500	Spheres
640	6.4	100	500	Spheres
2,270	22.7	200	500	Spheres

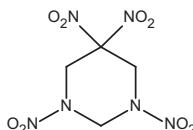
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1,3,5,5-Tetranitrohexahydropyrimidine

Name [German, acronym]: 1,3,5,5-Tetranitrohexahydro-1,3-diazine
[1,3,5,5-tetranitrohexahydropyrimidin, DNNC]

Main (potential) use: high explosive

Structural formula:



	DNNC		
Formula	$C_4H_6N_6O_8$		
Molecular mass [g mol ⁻¹]	266.13		
Appearance at RT	Colorless crystals ^[5] , small colorless, transparent rods on recryst. form EtOH ^[6]		
IS [J]	3.5 cm (ABL) ^[1] , Thiokol Corporation impact = 25.5 in ^[1]		
FS [N]	660 lb @ 8 ft/s (ABL) ^[1]		
ESD [J]	Thiokol Corporation ESD (unconfined) = 1.9, no bulk ignition ^[1]		
N [%]	31.6		
$\Omega(CO_2)$ [%]	-18.04		
$T_{m.p.}$ [°C]	153–154 ^[1, 7] , 152–154 ^[2] , 154.8–156.2 (DSC, 1.50–1.53 mg sample, melts without noticeable dec.) ^[4] , 151–154 ^[1, 6]		
$T_{phase\ transition}$ [°C]	195 K (first order phase transition below which, positioning of – NO ₂ groups causes lower molecular symmetry, FTIR) ^[5] , 1,965 K solid–solid phase transition DNNC-I (high temperature structure) – DNNC-II ^[5] , DNNC-I is stable for at least 1 h @ 193 K ^[5] , transformation of DNNC-I–DNNC-II is completely reversible @ ~ 195 K ^[5]		
$T_{dec.}$ [°C]	219 (onset), 227 (peak) (DSC) ^[1]		
ρ [g cm ⁻³]	1.82 ^[1]		
Heat of formation	11 kcal/mol (ΔH_f) ^[1]		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{ex}U^\circ$ [kJ kg ⁻¹]			
T_{ex} [K]			
p_{C-J} [kbar]			

VoD [m s ⁻¹]																														
V _o [L kg ⁻¹]																														
Thermal stability	IDSC analysis showing mass loss in the solid state dec. process ^[3] :																													
	<table><tr><th>T (°C)</th><th>Mass loss (%)</th><th>S.D.</th></tr><tr><td>148</td><td>78.5</td><td>± 5.1</td></tr><tr><td>145</td><td>75.5</td><td>± 3.3</td></tr><tr><td>142</td><td>75.2</td><td>± 1.5</td></tr></table>			T (°C)	Mass loss (%)	S.D.	148	78.5	± 5.1	145	75.5	± 3.3	142	75.2	± 1.5															
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	<table><tr><th>T (°C)</th><th>t_i (min)</th><th>S.D.</th><th>KDIE (t_d/t_h)</th></tr><tr><td>148</td><td>184</td><td>± 18</td><td>1.14</td></tr><tr><td>145</td><td>251</td><td>± 19</td><td>1.36</td></tr><tr><td>142</td><td>293</td><td>± 67</td><td>1.25</td></tr></table>			T (°C)	t _i (min)	S.D.	KDIE (t _d /t _h)	148	184	± 18	1.14	145	251	± 19	1.36	142	293	± 67	1.25											
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Solid state endothermic induction period activation energy = 128.1 kJ/mol ^[3] , liquid state endothermic induction period activation energy = 185.0 kJ/mol ^[3]																														
Physical properties of neat liquid DNNC thermochemical data ^[4] :																														
<table><tr><th>T (°C)</th><th>Induction time (s)</th><th>ΔH_{dec} (kJ mol⁻¹)</th><th>wt. loss (%)</th></tr><tr><td>194</td><td>52.6 ± 28.3</td><td>-802.5 ± 48.5</td><td>80 ± 2</td></tr><tr><td>190</td><td>72.2 ± 19.3</td><td>-775.3 ± 56.9</td><td>82 ± 4</td></tr><tr><td>186</td><td>93.8 ± 17.5</td><td>-801.6 ± 30.1</td><td>82 ± 4</td></tr><tr><td>182</td><td>148.4 ± 13.8</td><td>-786.6 ± 38.1</td><td>80 ± 5</td></tr><tr><td>178</td><td>228.6 ± 76.4</td><td>-799.1 ± 61.1</td><td>80 ± 7</td></tr><tr><td>174</td><td>359.6 ± 153.7</td><td>-803.3 ± 38.1</td><td>80 ± 3</td></tr></table>			T (°C)	Induction time (s)	ΔH _{dec} (kJ mol ⁻¹)	wt. loss (%)	194	52.6 ± 28.3	-802.5 ± 48.5	80 ± 2	190	72.2 ± 19.3	-775.3 ± 56.9	82 ± 4	186	93.8 ± 17.5	-801.6 ± 30.1	82 ± 4	182	148.4 ± 13.8	-786.6 ± 38.1	80 ± 5	178	228.6 ± 76.4	-799.1 ± 61.1	80 ± 7	174	359.6 ± 153.7	-803.3 ± 38.1	80 ± 3
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Vapor pressure [atm. @ °C]	5.27 × 10 ⁻⁷ mm Hg ^[1]																													
Burn rate [mm/s]	0.27 (@ 1 atm., SMATCH/FTIR spectroscopy) ^[8] , 0.27 (@ 1 atm., strand burner) ^[8]																													
Solubility [g/mL]	50,100 mg/L in H ₂ O (predicted) ^[1] , soluble in acetone, dichloromethane, acetonitrile and methyl acetate ^[5] , soluble in EtOH ^[6]																													
Photosensitivity	No photolysis expected ^[1]																													
Heat of fusion [kcal/mol]	5.19 ^[4]																													

SBAT [°F]	317 (onset) ^[1]
Log K_{ow}	−1.14 (predicted) ^[1] , $K_{ow} = 0.72 \text{ L/Kg}^{[1]}$
K_{oc}	1,678 (predicted) ^[1]
$\Delta H_{\text{phase transition}}$ [kcal/mol]	0.8 (DNNC-I \rightarrow DNNC-II) ^[5]

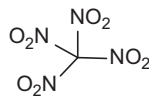
	DNNC ^[5]
Chemical formula	$\text{C}_4\text{H}_6\text{N}_6\text{O}_8$
Molecular weight [g mol ^{−1}]	266.02
Crystal system	Orthorhombic
Space group	$P2_12_12_1$ (no. 19)
a [Å]	11.130(2)
b [Å]	11.227(2)
c [Å]	15.705(3)
α [°]	90
β [°]	90
γ [°]	90
V [Å ³]	1,962.44
Z	8
ρ_{calc} [g cm ^{−3}]	1.801
T [K]	295

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Tetranitromethane

Name [German, acronym]: Tetranitromethane [tetranitromethan, TNM]
Main (potential) use: Possible oxidizer, explosive mixture component, component in detonating compositions and blasting explosives^[27], oxidizer in liquid-fueled rocks or as a monopropellant^[31]

Structural formula:



	TNM																								
Formula	CN ₄ O ₈																								
Molecular mass [g mol ⁻¹]	196.03																								
Appearance at RT	Colorless–pale yellow colored liquid ^[11, 25] , free-flowing, volatile, transparent and colorless liquid with a sharp odor ^[29] , colorless liquid with pungent odor ^[31] , pale yellow liquid ^[33] , colorless to pale yellow oily liquid ^[8] , freezes to colorless solid ^[11]																								
IS [J]	<p>$H_{50\%} \approx 100$ cm (2 kg mass, B.M.)^[11], $H_{50\%} = 320$ cm (2.5 kg mass, type 13 tool, ERL method)^[28], >320 cm (2.50 kg mass, ERL machine)^[35]</p> <p>IS of TNM mixtures with combustible materials (2.5 kg mass, ERL machine; reference sensitivities: NG = 4–5 cm, RDX = 22 cm, TNT = 160 cm, pure TNM ≈ 320 cm)^[35]:</p> <table><tr><th>Diluent</th><th>wt. % TNM</th><th>IS (cm)</th></tr><tr><td rowspan="4">NM</td><td>44.6</td><td>109</td></tr><tr><td>21.2</td><td>196</td></tr><tr><td>65</td><td>180</td></tr><tr><td>85</td><td>210</td></tr><tr><td rowspan="4">Nitrobenzene</td><td>42.6</td><td>264</td></tr><tr><td>61.7</td><td>44</td></tr><tr><td>76.3</td><td>22</td></tr><tr><td>82.8</td><td>47</td></tr><tr><td>2,4-Dinitrobutulene</td><td>95</td><td>300</td></tr></table>	Diluent	wt. % TNM	IS (cm)	NM	44.6	109	21.2	196	65	180	85	210	Nitrobenzene	42.6	264	61.7	44	76.3	22	82.8	47	2,4-Dinitrobutulene	95	300
Diluent	wt. % TNM	IS (cm)																							
NM	44.6	109																							
	21.2	196																							
	65	180																							
	85	210																							
Nitrobenzene	42.6	264																							
	61.7	44																							
	76.3	22																							
	82.8	47																							
2,4-Dinitrobutulene	95	300																							

FS [N]	$\geq 131 \text{ kPa} \times 10^{-4}$ @ 2.4 m/s (threshold level above which initiation occurs) ^[21] , 2/10 explosions in friction pendulum test ^[8]		
N [%]	28.58		
$\Omega(\text{CO}_2)$ [%]	+49.0		
$T_{\text{m.p.}}$ [°C]	13.8 ^[1, 33] , 14.2 ^[5, 8, 11] , 14.2 (freezing point) ^[29] , 13.5–13.8 (freezing point, technical product) ^[29] , 14 ^[31] , 14.136 (freezing point, 99.996% purity) ^[35]		
$T_{\text{b.p.}}$ [°C]	123.7 ^[25] , 126–127 (with partial dec.) ^[29] , 130 ^[31] , 126 (without dec.) ^[32] , bp ₇₆₀ = 126 ^[33] , bp _{25.8} = 40 ^[33] , bp _{14.9} = 30 ^[33] , bp _{8.4} = 20 ^[33] , bp _{5.7} = 13.8 ^[33] , bp _{1.9} = 0 ^[33] , 126 ^[8] , 125.7 ^[11] , 126 (760 mm Hg, 99.996% purity) ^[35]		
ρ [g cm ⁻³]	1.6377 ^[2, 8, 10] , 1.641 ^[3] , 1.650 (@ 286 K) ^[5] , 1.62294 (@ 25 °C) ^[11] , 1.65 ^[23] , 1.65 (@ TMD) ^[26] , sp. gr. $d^{15}_4 = 1.65$ ^[29] , 1.64 ^[31] , $d^{25}_4 = 1.6229$ ^[33] , $d^{25}_4 = 1.638$ (technical grade) ^[33] , 1.65 (99.996% purity) ^[35]		
Heat of formation	13.0 kcal mol ⁻¹ ^[6] , 38.40 kJ/mol (standard heat of form.) ^[8] , 196.4 kJ/kg (enthalpy of form.) ^[10] , 45 cal/g ^[3] , 195.89 kJ/kg (standard heat of form.) ^[8] , –8.9 kcal/mol ^[11] , 9.2 kcal/mol (liq., $\Delta_f H^\circ$) ^[22] , 19.7 kcal/mol ($\Delta_f H^\circ$ (gas)) ^[22] , –9.1 ± 0.4 kcal/mol ($\Delta_f H^\circ$ (liq.)) ^[19] , 19.7 ± 0.4 kcal/mol ($\Delta_f H^\circ$ (gas)) ^[19] , 8.8 kcal/mol ($\Delta_f H^\circ$) ^[20] , 54.39 kJ/mol ^[26] , 38.5 kJ/mol (enthalpy of form.) ^[31] , 25.6 kcal/mol ($\Delta H_f(g)^\circ$, calcd., ccCA-P) ^[34] , 22.0 kcal/mol ($\Delta H_f(g)^\circ$, calcd., ccCA-S3) ^[34] , –23.8 kcal/mol ($\Delta H_f(g)^\circ$, calcd., ccCA-PS3) ^[34] , 18.8 kcal/mol ($\Delta H_f(g)^\circ$, calcd., G3) ^[34] , 25.6 kcal/mol ($\Delta H_f(g)^\circ$, calcd., G3(MP2)) ^[34] , 19.7 ± 0.4 kcal/mol ($\Delta H_f(g)^\circ$, exptl.) ^[34]		
Heat of combustion	–2,217.5 J/g ^[8] , 102.9 kcal/mol ^[11] , $\Delta_c H^\circ = -103.2 \pm 0.4 \text{ kcal/mol}$ ^[19, 22]		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{\text{ex}} U^\circ$ [kJ kg ⁻¹]	2,255	55 kcal/g [H ₂ O (l)] (calcd.) ^[13] 55 kcal/g [H ₂ O (g)] (calcd.) ^[13] 552 cal/g ^[17] 45.6 kcal/100 g (@ 1.643 g cm ⁻³ , constant volume) [H ₂ O (l)] ^[30] 2,200 ^[31] 2,259 J/g (explosion heat) ^[8] –1,890 J/g (explosion enthalpy) ^[8]	2,259 ^[9] 2,200 ^[10] 557 cal/g (calcd. from DTA) ^[11] 580 kcal/kg ^[29]

T_{ex} [K]	2,570	<p>2,243 (@ 1.64 g cm⁻³, calcd.)^[20]</p> <p>2,222 (@ 1.65 g cm⁻³, calcd., KLRR/C, THEOSTAR-T)^[23]</p> <p>2,651 (@ 1.65 g cm⁻³, calcd., BKWC, THEOSTAR-T)^[23]</p> <p>2,112 (@ 1.65 g cm⁻³, calcd., BKWR, THEOSTAR-T)^[23]</p> <p>2,100 °C (@ 1.643 g cm⁻³)^[30]</p> <p>2,180 (@ 1.64 g cm⁻³, calcd. BKWR)^[6]</p> <p>2,860 (@ 1.64 g cm⁻³, calcd. BKWS)^[6]</p>	<p>2,800 (@ 1.64 g cm⁻³)^[6, 15]</p> <p>3,100^[15]</p> <p>2,900 °C^[29]</p>
$p_{\text{C-1}}$ [kbar]	145	<p>144 (calc.)^[5]</p> <p>159 (@ 1.64 g cm⁻³, calcd., Xiong)^[17]</p> <p>147.9 (@ 1.64 g cm⁻³, calcd.)^[20]</p> <p>15.1 GPa (@ 1.65 g cm⁻³, calcd., KLRR/C, THEOSTAR-T)^[23]</p> <p>13.8 GPa (@ 1.65 g cm⁻³, calcd., BKWC, THEOSTAR-T)^[23]</p> <p>14.8 GPa (@ 1.65 g cm⁻³, calcd., BKWR, THEOSTAR-T)^[23]</p> <p>1.44×10^7 Pa^[8]</p> <p>150 (@ 1.64 g cm⁻³, calcd., BKWR)^[6]</p> <p>116 (@ 1.64 g cm⁻³, calcd., BKWS)^[6]</p>	<p>159 (@ 1.64 g cm⁻³)^[6, 15, 17]</p> <p>159^[14]</p> <p>15.5 GPa (@ 1.65 g cm⁻³)^[23]</p>

VoD [m s ⁻¹]	6,367 (@ TMD)	6,750 (@ 1.65 g cm ⁻³ (TMD), calcd., R-P method) ^[16] 6,270 (@ 1.65 g cm ⁻³ (TMD), calcd., <i>Aizenshtadt</i>) ^[16] 6,670 (@ 1.65 g cm ⁻³ (TMD), calcd., K- <i>J</i>) ^[16] 6,446 (@ 1.64 g cm ⁻³ , calcd., <i>Xiong</i>) ^[17] 6,410 (@ 1.64 g cm ⁻³ , calcd.) ^[20] 6,460 (@ 1.65 g cm ⁻³ , calcd., KLRR/C, THEOSTAR-T) ^[23] 6,260 (@ 1.65 g cm ⁻³ , calcd., BKWC, THEOSTAR-T) ^[23] 6,180 (@ 1.65 g cm ⁻³ , calcd., BKWR, THEOSTAR-T) ^[23] 6,360 (@ 1.64 g cm ⁻³ , confined) ^[31] 6,220 (@ 1.64 g cm ⁻³ , calcd. BKWR) ^[6] 5,540 (@ 1.64 g cm ⁻³ , calcd. BKWS) ^[6]	6,360 (@ 1.64 g cm ⁻³) ^[4, 6, 15, 17] 6,400 (@ 1.6 g cm ⁻³) ^[5, 13] 6,360 (@ 1.637 g cm ⁻³) ^[10] 6,400 (@ 1.65 g cm ⁻³) ^[18] 6.55 mm/μs (@ TMD) ^[14] 6,400 (@ 1.64 g cm ⁻³) ^[20] 6,450 (@ 1.65 g cm ⁻³) ^[23]
V ₀ [L kg ⁻¹]	744	68.6 l/100 g (@ 1.643 g cm ⁻³ , @ STP) ^[30]	685 ^[7, 9, 10] 670 ^[29]

Data from^[26]:

Initial density (g/cm ³)	Inner diameter (mm)	Wall thickness (mm)	Wall velocity (mm/μs) at 25.4 mm diameter for R-R ₀ equal to			Velocity-squared cf. with PETN for the same configuration, % comparison R-R ₀ equal to		
			6 mm	12.5 mm	19 mm	6 mm	12.5 mm	19 mm
1.650	25.43	2.592	1.000	1.095	1.130	-58.9	-58.8	-60.1

Summary of code calculations with measure detonation velocities and detonation energies derived from JWL's^[26]:

Initial density (g/cm ³)	PETN-adjusted BKWR Tiger, LLNL library, $\theta = 1,850$ K, at v			JCZ3, LLNL library, v			CHEQ V2.4, at v		
	2.2 mm	4.1 mm	6.5 mm	2.2 mm	4.1 mm	6.5 mm	2.2 mm	4.1 mm	6.5 mm
1.65	2	-1	1	5	0	1	-1	-4	-2

JWL cylinder coefficients data from^[26]:

Initial density, ρ_0 (g/cm ³)	Detonation velocity, D (mm/ μ s)	Energy of detonation, E_0 (kJ/cm ³)	CJ pressure (GPa)	A (GPa)	B (GPa)	C (GPa)	R_1	R_2	ω	γ_{CJ}
1.65	6.45	-3.60	15.5	642.2267	3.898275	0.258200	5.020	0.90	0.52	3.429

Comparison of measured "CJ" temperatures using optical pyrometry^[26]:

Experimental density (g/cm ³)	Max. measured T (K)	Calculated CJ T (K)			Wavelength (μ m)
		Tiger BKWR	Tiger JCZ3	CHEQ	
1.64	2,840	2,200	2,500	2,500	0.6-0.9

Critical diameter [cm]	d_c for detonation propagation of TNM thickened with poly(methylacrylate) and loaded with up to 75% inert solids decreased with increasing solids loading ^[11]
Trauzl test [cm ³ , % TNT]	21.4% TNT (when pure TNM) ^[8, 11] , 54% TNT ^[18] , 134% TNT (87:13 mixture with benzene) ^[11] , 30.62 cc (4 moles NMe:1 mole TMN) ^[11]
Sand test [g]	108% TNT ^[18] , 7.5 g ^[8]
Initiation efficiency	Not fully detonated by 10 g Tetryl ^[8]
Gap test	>300 cards (mixture of 65-90% in benzene) ^[11] , 270 cards (50% soln. by weight in ethylene glycol) ^[11] , 75 cards (mixture with NM containing 40% TNM) ^[11]
5 s explosion T [°C] 5 s flash point [°C] Explosion T [°C]	225 ^[8] Does not explode below 360 °C ^[11]
100 °C heat test [% mass loss]	Acid fumes produced within 30 minutes ^[11] , no explosion after 300 min @ 135 °C ^[11]

Vacuum stability test [cm ³ /h]	No gas released from 2.5 g sample @ 90 °C for 6 h ^[8]
Thermal stability	Becomes acidic on standing due to dec. ^[29] , dec. more readily in presence of water ^[29] , stable in acidic media and can be stored in these conditions for years ^[29] , stable on storage @ 25 °C ^[32]
Vapor pressure [atm. @ °C]	13 mm Hg @ 25 °C ^[13]
Enthalpy of vaporization [kcal mol ⁻¹]	10.6 ± 0.1 ^[19]
Heat of fusion [cal/mol]	2,250.6 ^[35]
Viscosity [cP]	0.0177 Poise @ 20 °C ^[29] , 1.76 cP @ 20 °C ^[33]
Solubility [g/mL]	Insoluble in water ^[8, 25, 31, 33] , very soluble in EtOH, Et ₂ O and hydrocarbons ^[25] , virtually insoluble in water, glycerol ^[29] , readily soluble in toluene, benzene, dichloroethane and many other common organic solvents ^[29] , TNT, paraffin and naphthalene are miscible with tetranitromethane in any ratio @ <i>T</i> above their mpts. ^[29] , soluble in sulfuric and nitric acids ^[29] , freely soluble in EtOH, Et ₂ O and alcoholic KOH ^[33] , soluble in many organic solvents, e.g., EtOH, Et ₂ O, acetone, toluene, nitrobenzene ^[8]
Hygroscopicity	Nonhygroscopic ^[29]
Compatibility	Forms explosive mixtures with wood, oil, grease or other organic materials ^[25] , technical product is stabilized by sulfuric acid or nitrogen oxides (to an acidity of 0.1–0.2%) which allows storage in iron apparatus ^[29] , attacks iron, copper, brass, zinc, rubber ^[33] , pure TNM is colorless but becomes yellow on contact with water due to hydrolysis ^[11]
Activation energy of thermal decomposition [kJ/mol]	$E_{A \text{ soln.}} = 173.0$ (Freon 114B) ^[24] , $E_{A \text{ soln.}} = 166.3$ (CCl ₄) ^[24] , $E_{A \text{ gaseous}} = 160.1$ ^[24] , $E_{A \text{ calcd.}} = 168$ ^[24]
Refractive index	$n_D^{20} = 1.4384$ ^[33] , $n_D^{25} = 1.4358$ ^[33] , 1.4382225 ^[8] , 1.43822 @ 25 °C ^[11] , $n_D^{25} = 1.4351$ (99.996% purity) ^[35]
Dipole moment [D]	Essentially zero ^[11]

	C(NO₂)₄ ^[12]	C(NO₂)₄ ^[12]
Chemical formula	CN ₄ O ₈	CN ₄ O ₈
Molecular weight [g mol ⁻¹]	196.05	196.05
Crystal system	Orthorhombic	Tetragonal

Space group	$Pca2_1$	$I \bar{4}$ (no. 82)
a [Å]	9.7331(2)	6.9893(3)
b [Å]	9.7317(2)	6.9893(3)
c [Å]	20.4635(5)	6.9866(7)
α [°]	90	90
β [°]	90	90
γ [°]	90	90
V [Å ³]	1,938.28(7)	341.30(4)
Z	12	2
ρ_{calc} [g cm ⁻³]	2.016	1.908
T [K]	100	200

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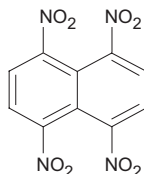
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Tetranitronaphthalene

Name [German, acronym]: Tetranitronaphthalene, 1,4,5,8-tetranitronaphthalene [tetranitronaphthalin, TNN, TENN, 1,4,5,8-TENN, β -TENN]

Main (potential) use: Investigated as possible heat-resistant explosive, used in dynamites, safety explosives and as a component of some military explosives^[16]

Structural formula:



	TNN
Formula	C ₁₀ H ₄ N ₄ O ₈
Molecular mass [g mol ⁻¹]	308.16
Appearance at RT	Sand colored crystals ^[17] , yellowish solid (mixture of isomers) ^[20]
IS [J]	9.64 (first reaction) ^[5, 18] , 24.61 (sound) ^[5, 18] , $H_{50\%} = 99$ cm (2.5 kg mass, sandpaper, NOL apparatus) ^[9] , 9.65 (drop energy, Julius-Peters apparatus) ^[10] , $H_{50} = 100$ cm (2.5 kg mass, type 12 tool) ^[19]
ESD [J]	8.26 ^[3, 25] , 95.0 mJ ^[3] , 8.26 (for <i>para</i> isomer) ^[4]
<i>N</i> [%]	18.18
$\Omega(\text{CO}_2)$ [%]	-72.7
$T_{\text{phase transitions}}$ [°C]	250–260 ^[9]
$T_{\text{m.p.}}$ [°C]	207 ^[1] , 190 (softening of the isomer mixture) ^[7] , >450 (dec. without melting) ^[9] , 450 ^[11] , 340–350 (with dec., 1,4,5,8-isomer) ^[9] , 203 (1,3,6,8-isomer, β -isomer) ^[16, 17] , 194–195 (1,3,5,8-isomer, γ -isomer) ^[16, 17] , 270 (dec., no melting, 1,2,5,8-isomer) ^[16] , 340–345 (1,4,5,8-isomer) ^[17] , 260 (1,3,5,7-isomer) ^[17] , 205–220 (mixture of isomers) ^[20]
$T_{\text{dec.}}$ [K]	579 (DTA, onset) ^[3, 18] , >450 °C (dec. without melting) ^[9]
ρ [g cm ⁻³]	1.8 ^[7, 8] , 1.802 (@ 293 K) ^[2] , 1.80 (crystal) ^[9] , 1.823 (X-ray @ 295 K, Form-II) ^[15]
Heat of formation	12.9 kcal mol ⁻¹ (ΔH° , exptl.) ^[8] , 11.3 ± 2.0 kcal/mol (ΔH_f°) ^[8] , 35.3 kJ/kg (enthalpy of form.) ^[7] , -32.5 kcal/kg ^[22] , 10.8 kJ/mol (enthalpy of form., exptl.) ^[24] , 1.3 kJ/mol (enthalpy of form., calcd., emp.) ^[24] , 47.8 kJ/mol (enthalpy of form., calcd., S-D method) ^[24]

Heat of combustion	$\Delta H_c^\circ = -1,090.0$ kcal/mol (exptl.) ^[8] , 3,522 kcal/kg (@ C ^V) ^[22]		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^\circ$ [kJ kg ⁻¹]	4,449		2,887 [H ₂ O (g)] ^[6]
T_{ex} [K]	3,303		
$p_{\text{C-J}}$ [kbar]	216	236 (calcd., K-J) ^[8]	25.74 GPa (1,4,5,8-isomer) ^[21]
VoD [m s ⁻¹]	7,206	7,300 (@ 1.88 g cm ⁻³ , calcd., K-J) ^[8]	7,013 in 1/4 in Al tubes ^[9]
V_0 [L kg ⁻¹]	574		780 ^[9]

Ballistic mortar test	101% TNT ^[12]
Vacuum stability test [cm ³ /h]	0.22 cc/g/h gas evolved @ 280 °C ^[9] , 1.1 cc/g/h @ 300 °C ^[9] @ 200 °C (total vol. of gas evolved (cm ³)/no. of days): 0.3/2, 0.5/7, 0.6/14, 0.8/21, 0.9/28, 1.0/35, 1.2/42, 1.3/49, 1.4/56, 1.6/63, 1.7/70, 1.8/77, 2.0/84, 2.2/91 ^[13, 23]
Solubility [g/mL]	All isomers are poorly soluble in common organic solvents ^[17] , 1,3,5,8-isomer is readily soluble in acetone ^[17]

	1,3,6,8-TNN ^[14]	1,3,6,8-TNN ^[14]	1,3,6,8-TNN ^[14]
Chemical formula	C ₁₀ H ₄ N ₄ O ₈	C ₁₀ H ₄ N ₄ O ₈	C ₁₀ H ₄ N ₄ O ₈
Molecular weight [g mol ⁻¹]	308.16	308.16	308.16
Crystal system	Orthorhombic	Orthorhombic	
Space group	<i>Pbn</i> (no. 562)	<i>P2₁2₁2₁</i> (no. 19)	
<i>a</i> [Å]	7.77	8.87	16.4
<i>b</i> [Å]	26.4	26.5	29.6
<i>c</i> [Å]	5.55	7.16	7.56
α [°]	90	90	90
β [°]	90	90	90
γ [°]	90	90	90
<i>V</i> [Å ³]	1,138.46	1,682.99	3,669.93

Z	4		
ρ_{calc} [g cm ⁻³]	1.798		
T [K]	295	295	295

	1,4,5,8-TNN^[15] (Form-II)
Chemical formula	C ₁₀ H ₄ N ₄ O ₈
Molecular weight [g mol ⁻¹]	308.16
Crystal system	Monoclinic
Space group	$P2_1/c$ (no. 14)
a [Å]	5.38
b [Å]	7.71
c [Å]	13.55
α [°]	90
β [°]	92.7
γ [°]	90
V [Å ³]	561.427
Z	2
ρ_{calc} [g cm ⁻³]	1.823
T [K]	295
Comments	RT stable polymorph

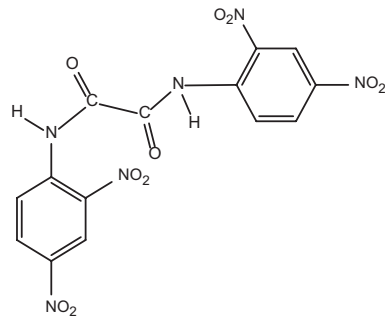
- [1] “PhysProp” data were obtained from Syracuse Research Corporation of Syracuse, New York (US)
- [2] Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994–2017 ACD/Labs).
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2,4,2',4'-Tetranitrooxanilide

Name [German, acronym]: *N,N'*-Di-(2,4-dinitrophenyl)ethanediamide [TNO]
 Main (potential) use: Component of black powder type and pyrotechnic compositions^[2]

Structural formula:



	TNO		
Formula	C ₁₄ H ₈ N ₆ O ₁₀		
Molecular mass [g mol ⁻¹]	420.25		
Appearance at RT	light yellow solid ^[2]		
IS [J]	30 in (P.A.) ^[1] , 30 in (2 kg mass, 11 mg sample, P.A.) ^[2] , 18 in (2 kg mass, P.A., height of first indication of no detonation, confined sample) ^[3]		
FS [N]	Unaffected by steel shoe (friction pendulum test) ^[2] , unaffected by fiber shoe (friction pendulum test) ^[2]		
N [%]	20.00		
Ω(CO ₂) [%]	-84		
T _{m,p.} [°C]	313 ^[1] , 313 (dec.) ^[2, 4]		
T _{dec.} [°C]			
ρ [g cm ⁻³]			
Heat of formation			
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
-Δ _{ex} U° [kJ kg ⁻¹]			
T _{ex} [K]			

p_{C-J} [kbar]			
VoD [m s ⁻¹]			
V_0 [L kg ⁻¹]			
Sand test [g]	16.3 g (20 g bomb) ^[2]		
Initiation efficiency	0.20 g LA minimum detonating charge ^[2] , 0.25 g Tetryl minimum detonating charge ^[2]		
5 s explosion T [°C]	392 ^[1, 2]		
100 °C heat test [% mass loss]	0.07% in first 48 h ^[1, 2] , 0.00% in second 48 h ^[1, 2] , no explosions in 100 h ^[2]		
Vacuum stability test [cm ³ /h]	0/40 (@ 90 °C) ^[1] , 0/40 (@ 100 °C) ^[1] , 0.11/40 (@ 120 °C) ^[1, 2]		
Solubility [g/mL]	<0.10% in water @ 100 °C ^[2] , 715% in nitrobenzene @ 150 °C ^[2] , insoluble in EtOH ^[2] , insoluble in benzene ^[2] , insoluble in butyl acetate ^[2] , insoluble in CCl ₄ ^[2] , insoluble in ethyl ether ^[2] , soluble in acetic acid ^[2] , soluble in nitric acid ^[2] , soluble in caustic potash ^[2] , very soluble in DMF ^[2]		
Hygroscopicity	Trace @ 30 °C with 90% RH ^[2]		

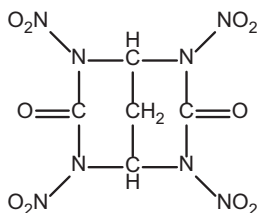
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2,4,6,8-Tetranitro-2,4,6,8-tetraazabicyclo[3.3.1]nonane-3,7-dione

Name [German, acronym]: Tetranitropropane diurea [TNPDU]

Main (potential) use: Possible future thermally stable, insensitive explosive^[1]

Structural formula:



	TNPDU														
Formula	C ₅ H ₄ N ₈ O ₁₀														
Molecular mass [g mol ⁻¹]	336.13														
Appearance at RT	White solid ^[1]														
IS [J]	<p>$H_{50\%} = 27.5$ cm (2 kg mass, Bruceton method)^[1]</p> <p>Height for 50% explosion, 2 kg mass^[1]:</p> <table border="1"> <thead> <tr> <th>Composition</th><th>Height for 50% explosion (cm)</th></tr> </thead> <tbody> <tr> <td>TNPDU</td><td>20</td></tr> <tr> <td>TNPDU/Polyurethane, 90/10</td><td>25</td></tr> <tr> <td>TNPDU/Polyurethane, 85/15</td><td>26</td></tr> <tr> <td>TNPDU/Polyurethane, 80/20</td><td>40</td></tr> <tr> <td>TNPDU/Paraffin wax, 90/10</td><td>26</td></tr> <tr> <td>TNPDU/Paraffin wax, 85/15</td><td>47</td></tr> </tbody> </table>	Composition	Height for 50% explosion (cm)	TNPDU	20	TNPDU/Polyurethane, 90/10	25	TNPDU/Polyurethane, 85/15	26	TNPDU/Polyurethane, 80/20	40	TNPDU/Paraffin wax, 90/10	26	TNPDU/Paraffin wax, 85/15	47
Composition	Height for 50% explosion (cm)														
TNPDU	20														
TNPDU/Polyurethane, 90/10	25														
TNPDU/Polyurethane, 85/15	26														
TNPDU/Polyurethane, 80/20	40														
TNPDU/Paraffin wax, 90/10	26														
TNPDU/Paraffin wax, 85/15	47														
FS [N]	<p>Insensitive up to 8 kg (Julius-Peters apparatus)^[1]</p> <p>Insensitive up to (kg)^[1]:</p> <table border="1"> <thead> <tr> <th>Composition</th><th>FS (kg)</th></tr> </thead> <tbody> <tr> <td>TNPDU</td><td>8</td></tr> <tr> <td>TNPDU/Polyurethane, 90/10</td><td>12</td></tr> <tr> <td>TNPDU/Polyurethane, 85/15</td><td>19.2</td></tr> <tr> <td>TNPDU/Polyurethane, 80/20</td><td>16</td></tr> <tr> <td>TNPDU/Paraffin wax, 90/10</td><td>21.6</td></tr> <tr> <td>TNPDU/Paraffin wax, 85/15</td><td>36</td></tr> </tbody> </table>	Composition	FS (kg)	TNPDU	8	TNPDU/Polyurethane, 90/10	12	TNPDU/Polyurethane, 85/15	19.2	TNPDU/Polyurethane, 80/20	16	TNPDU/Paraffin wax, 90/10	21.6	TNPDU/Paraffin wax, 85/15	36
Composition	FS (kg)														
TNPDU	8														
TNPDU/Polyurethane, 90/10	12														
TNPDU/Polyurethane, 85/15	19.2														
TNPDU/Polyurethane, 80/20	16														
TNPDU/Paraffin wax, 90/10	21.6														
TNPDU/Paraffin wax, 85/15	36														

N [%]	33.34																										
$\Omega(\text{CO}_2)$ [%]	−9.52																										
$T_{\text{m.p.}}$ [°C]	>220 (deflagration, recryst.) ^[1]																										
$T_{\text{dec.}}$ [°C]	194 (exo, onset), 220 (exo peak max), (DTA) ^[1] , 235 (DTA) ^[1] DTA data from ^[1] (magnitude of exothermicity is ratio of peak height to mass of sample): <table><tr><td>Compound/mixture</td><td>T_i (°C)</td><td>T_m (°C)</td><td>Exothermicity</td></tr><tr><td>TNPDU</td><td>194</td><td>220</td><td>10.5</td></tr><tr><td>TNPDU + NTO</td><td>220</td><td>240</td><td>10</td></tr><tr><td>TNPDU + ANTA</td><td>220</td><td>245</td><td>3.9</td></tr><tr><td>TNPDU + TATB</td><td>218</td><td>235</td><td>3.57</td></tr><tr><td>TNPDU + TNABN</td><td>199</td><td>220</td><td>2.65</td></tr></table>			Compound/mixture	T_i (°C)	T_m (°C)	Exothermicity	TNPDU	194	220	10.5	TNPDU + NTO	220	240	10	TNPDU + ANTA	220	245	3.9	TNPDU + TATB	218	235	3.57	TNPDU + TNABN	199	220	2.65
Compound/mixture	T_i (°C)	T_m (°C)	Exothermicity																								
TNPDU	194	220	10.5																								
TNPDU + NTO	220	240	10																								
TNPDU + ANTA	220	245	3.9																								
TNPDU + TATB	218	235	3.57																								
TNPDU + TNABN	199	220	2.65																								
ρ [g cm ^{−3}]	1.93 (exptl.) ^[1]																										
Heat of formation	−81.39 kJ/mol (ΔH_f , calcd.) ^[1]																										
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.																								
− $\Delta_{\text{ex}}U^\circ$ [kJ kg ^{−1}]																											
T_{ex} [K]																											
$p_{\text{C-J}}$ [kbar]		39.38 GPa (calcd.) ^[1]																									
VoD [m s ^{−1}]		9,034 (@ 1.93 g cm ^{−3} , calcd., R-P method) ^[1]																									
V_0 [L kg ^{−1}]																											
5 s explosion T [°C] Deflagration T [°C] Explosion delay T [°C]	252 (0.02 g sample, Wood's metal bath @ 5 °C/min) ^[1] Explosion delay measurements ^[1] : <table><tr><td>T (°C)</td><td>Explosion delay (s)</td></tr><tr><td>220</td><td>12.0</td></tr><tr><td>230</td><td>9.4</td></tr><tr><td>240</td><td>7.4</td></tr><tr><td>250</td><td>6.8</td></tr></table>			T (°C)	Explosion delay (s)	220	12.0	230	9.4	240	7.4	250	6.8														
T (°C)	Explosion delay (s)																										
220	12.0																										
230	9.4																										
240	7.4																										
250	6.8																										

Thermal stability	High thermal stability ^[1]			
Vacuum stability test [cm ³ /h]	Compatibility of vacuum stability data: @ 94 °C for 48 h/5 g, values in parentheses indicate the vacuum stabilities of the additional component, i.e. ANTA, TATB, TNABN and NTO ^[1] :			
	Composition	Vacuum stability @ 94 °C for 48 h, mL/5 g		
	TNPDU (crystalline)	0.7597		
	TNPDU (amorphous)	0.6191		
	TNPDU:ANTA (1:1)	0.4929 (0.3104)		
	TNPDU:TATB (1:1)	0.4369 (0.206)		
	TNPDU:TNABN (1:1)	0.5245 (0.3395)		
	TNPDU:NTO (1:1)	0.4098 (0.2139)		
Solubility [g/mL]	Recryst. from nitromethane ^[1]			
Compatibility	Better hydrolytic stability than similar compounds (e.g., TNGU) ^[1] , stable in neutral and acidic media ^[1] , immediate dec. in alkaline media (e.g. 0.1 M NaOH) ^[1] , compatible with ANTA, TATB, NTO and TNABN (see vacuum stability test data) ^[1]			
	DTA data from (magnitude of exothermicity is ratio of peak height to mass of sample) ^[1] :			
	Compound/mixture	T _i (°C)	T _m (°C)	Exothermicity
	TNPDU	194	220	10.5
	TNPDU + NTO	220	240	10
	TNPDU + ANTA	220	245	3.9
	TNPDU + TATB	218	235	3.57
	TNPDU + TNABN	199	220	2.65

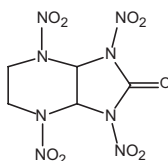
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2,5,7,9-Tetranitro-2,5,7,9-tetraazabicyclo[4.3.0]nonane-8-one

Name [German, acronym]: 2,5,7,9-Tetranitro-2,5,7,9-tetraazabicyclo [4.3.0]nonane-8-one [K-56, TN650, TNABN]

Main (potential) use: Possible future thermally stable insensitive explosive^[6]

Structural formula:



	K-56		
Formula	$C_5H_6N_8O_9$		
Molecular mass [g mol ⁻¹]	322.15		
Appearance at RT	Needle crystals ^[3] , white crystals (recryst. from nitromethane) ^[6] , white powder ^[7] , white microcrystals (recryst. from EtOAc/toluene) ^[7]		
IS [J]	$H_{50} = 115$ cm (2 kg mass) ^[3] , $H_{50\%} = 20$ cm (Holston impact) ^[3] , 115 cm ^[4, 5] , $H_{50\%} = 115$ cm (2 kg mass, Bruceton method) ^[6]		
FS [N]	132.5 (50% value) ^[3] , insensitive up to 36 kg (Julius-Peters apparatus) ^[6]		
N [%]	34.78		
$\Omega(CO_2)$ [%]	-19.87		
$T_{m.p.}$ [°C]	>230 ^[4, 5, 6] , 194–196 (crystals) ^[6] , 203–204 (microcrystals recryst. from EtOAc/toluene) ^[7] , 194–196 (Thomas Hoover capillary apparatus) ^[8]		
$T_{dec.}$ [°C]	235 (DTA) ^[6] , 199 (onset), 205 (peak max) (DTA) ^[6]		
ρ [g cm ⁻³]	1.969 ^[1, 2] , 1.97 ^[3] , 1.92 ^[4–6] , 1.969 (X-ray) ^[7]		
Heat of formation	71.1 kJ/mol ($\Delta_f H^\circ$) ^[2] , 70.31 kJ/mol (ΔH) ^[3] , 70.313 kJ/mol (ΔH_f) ^[6]		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{ex}U^\circ$ [kJ kg ⁻¹]	5,661 ($\Delta H_f = 71$ kJ/mol, $\rho = 1.96$ g cm ⁻³)		
T_{ex} [K]	3,745 ($\Delta H_f = 71$ kJ/mol, $\rho = 1.96$ g cm ⁻³)		
p_{C-J} [kbar]	382 ($\Delta H_f = 71$ kJ/mol, $\rho = 1.96$ g cm ⁻³)	37.0 GPa (calcd.) ^[6]	

VoD [m s^{-1}]	9,169 ($\Delta H_f = 71 \text{ kJ/mol}$, $\rho = 1.96 \text{ g cm}^{-3}$)	9,015 (ρ not specified) ^[4, 5] 9,015 (@ 1.92 g cm^{-3} , calcd., R-P method) ^[6]	
V_0 [L kg^{-1}]	710 ($\Delta H_f = 71 \text{ kJ/mol}$, $\rho = 1.96 \text{ g cm}^{-3}$)		
5 s explosion T [$^{\circ}\text{C}$] Deflagration T [$^{\circ}\text{C}$]	202 (0.2 g sample, Wood's metal bath, @ 5°C/min) ^[6]		
Burn rate [mm/s]	Pressure interval = 0.1–4 MPa, pressure exponent = 0.547, burning rate = 26.5 mm/s @ 10 MPa, strand $\rho = 1.55 \text{ g/cc}$, adiabatic flame $T = 3,413 \text{ K}$ ^[2]		
Solubility [g/mL]	Recryst. from nitromethane ^[6]		

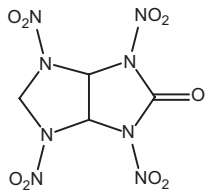
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2,4,6,8-Tetranitro-2,4,6,8-tetraazabicyclo[3.3.0]octane-3-one

Name [German, acronym]: 2,4,6,8-Tetranitro-2,4,6,8-tetraazabicyclo [3.3.0]octane-3-one [K-55, TN550]

Main (potential) use: high explosive

Structural formula:



	K-55		
Formula	C ₄ H ₅ N ₈ O ₉		
Molecular mass [g mol ⁻¹]	309.14		
Appearance at RT			
IS [J]			
FS [N]			
ESD [J]			
N [%]	36.37		
Ω(CO ₂) [%]	-7.76		
T _{m,p.} [°C]			
T _{dec.} [°C]			
ρ [g cm ⁻³]	1.91 (crystal) ^[1-3] , 1.954 ^[2]		
Heat of formation	23.0 kJ/mol (Δ _f H°) ^[2]		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
-Δ _{ex} U° [kJ kg ⁻¹]	5,924		
T _{ex} [K]	4,027		
p _{C-J} [kbar]	376		
VoD [m s ⁻¹]	9,183		
V ₀ [L kg ⁻¹]	745		

Burn rate [mm/s]	0.1–10.1 MPa pressure interval, pressure exponent = 0.901, burning rate @ 10 MPa = 63.1 mm/s, strand ρ = 1.72 g/cc, adiabatic flame T = 3,469 K ^[2]
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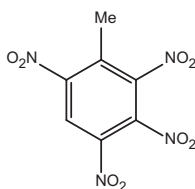
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Tetranitrotoluene

Name [German, acronym]: 2,3,4,6-Tetranitrotoluene,
2,3,4,6-tetranitromethylbenzene
[2,3,4,6-tetranitrotoluol, tetranitrotoluol, TeNT]

Main (potential) use: high explosive

Structural formula:



	TeNT
Formula	$C_7H_4N_4O_8$
Molecular mass [g mol ⁻¹]	272.13
Appearance at RT	Orange crystalline solid ^[7]
IS [J]	50 cm (2 kg mass) ^[1, 2] , H_{50} = 19 cm (2.5 kg mass, type 12 tool) ^[4] , H_{50} = 13 cm (2,3,4,5-) ^[5] , $H_{50\%}$ = 15 cm (2.5 kg, type 12 tool, B.M., 2,3,4,5-) ^[6] , $H_{50\%}$ = 19 cm (2.5 kg, type 12 tool, B.M., 2,3,4,6-) ^[6] , $H_{50\%}$ = 25 cm (2.5 kg, type 12 tool, B.M., 2,3,5,6-) ^[6] , 50 cm (2 kg mass, Kast apparatus) ^[7] , H_{50} = 25 cm (2,3,4,6-) ^[8] , H_{50} = 13 cm (2,3,4,5-) ^[8] , $H_{50\%}$ = 15 cm (2.5 kg mass, 2,3,4,5-isomer) ^[10] , $H_{50\%}$ = 19 cm (2.5 kg mass, 2,3,4,6-isomer) ^[10] , $H_{50\%}$ = 25 cm (2.5 kg mass, 2,3,5,6-isomer) ^[10]
N [%]	20.59
$\Omega(CO_2)$ [%]	-47.03
$T_{m.p.}$ [°C]	136.5 ^[1, 2, 7] , 135 ^[7] , 107–109 (2,3,4,5-isomer recryst.) ^[11] , 95–102 (crude, 2,3,4,5-isomer) ^[11] , 135–136.5 (2,3,4,6-isomer) ^[11] , 163–165 (2,3,5,6-isomer, double recryst.) ^[11] , 141–163 (crude, 2,3,5,6-isomer) ^[11] , 150–152 (2,3,5,6-isomer) ^[11]
$T_{dec.}$ [°C]	
ρ [g cm ⁻³]	1.72 (calcd., 2,3,4,5-, 2,3,4,6-, 2,3,5,6-) ^[6] , 1.71 (2,3,4,5-) ^[6] , 1.71 (2,3,4,6-) ^[6] , 1.69 (2,3,5,6-) ^[6] , 1.70 (2,3,4,5-isomer, gas pycnometer) ^[11] , 1.69 (2,3,4,6-isomer, gas pycnometer) ^[11] , 1.66 (2,3,5,6-isomer, gas pycnometer) ^[11]
Heat of formation	-34.0 kcal/mol (ΔH_f (g) @ 25 °C, 2,3,4,5-isomer, calcd., MINDO/3) ^[9] , -30.8 kcal/mol (ΔH_f (g) @ 25 °C, 2,3,4,6-isomer, calcd., MINDO/3) ^[9] , -30.0 kcal/mol (ΔH_f (g) @ 25 °C, 2,3,5,6-isomer, calcd., MINDO/3) ^[9]

	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^{\circ}$ [kJ kg ⁻¹]			
T_{ex} [K]			
$p_{\text{C-J}}$ [kbar]		256 (@ 1.73 g cm ⁻³ , 2,3,4,5-, calcd.) ^[6] 256 (@ 1.73 g cm ⁻³ , 2,3,4,6-, calcd.) ^[6] 256 (@ 1.73 g cm ⁻³ , 2,3,5,6-, calcd.) ^[6]	
VoD [m s ⁻¹]		7,600 (@ 1.73 g cm ⁻³ , 2,3,4,5-, calcd.) ^[6] 7,600 (@ 1.73 g cm ⁻³ , 2,3,4,6-, calcd.) ^[6] 7,600 (@ 1.73 g cm ⁻³ , 2,3,5,6-, calcd.) ^[6]	
V_0 [L kg ⁻¹]			
Trauzl test [cm ³ , % TNT]	327 cm ³ ^[1, 2] , 327 cm ³ (10 g sample) ^[7]		
Thermal stability	Turns yellow after 1 day ^[2] , 57% dec. @ 80 °C for 24 h ^[1] , tetranitrotoluenes are thermally stable and can be stored indefinitely at ambient T under anhydrous conditions like α -TNT ^[11]		
Solubility [g/mL]	Soluble in CHCl ₃ ^[7] , very slightly soluble in water ^[7]		
Dipole moment, μ [D]	6.19 (calcd., 2,3,4,5-TeNT) ^[3] , 0.93 (calcd., 2,3,5,6-TeNT) ^[3] , 3.54 (calcd., 2,3,4,6-TeNT) ^[3] , 6.55 (gas @ 25 °C, calcd., MINDO/3, 2,3,4,5-isomer) ^[9] , 3.85 (gas @ 25 °C, calcd., MINDO/3, 2,3,4,6-isomer) ^[9] , 1.23 (gas @ 25 °C, calcd., MINDO/3, 2,3,5,6-isomer) ^[9]		

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- [2] A. F. Holleman, *Chem. Zentralblatt*, **1930**, *D Org. Chem.*, Band II, 548.
- [3] P. Politzer, *Computational Studies of Polynitroaromatic Molecules and the Development of Sensitivity Relationships*, AFATL-TR-90-66, Air Force Armament Laboratory, Florida, USA, October **1990**.
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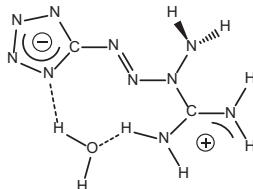
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- [11] A. T. Nielsen, S. L. Christian, A. P. Chafin, W. S. Wilson, *J. Org. Chem.*, **1994**, 59, 1714–1718.

Tetrazene*

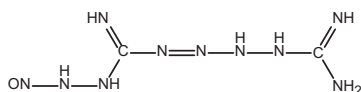
Name [German, acronym]: Tetrazene, 1-amino-1-((1*H*.tetrazol-5-yl)-azo)guanidine monohydrate, 4-guanyl-1-(nitrosoaminoguanyl)-1-tetrazene, 1-amino-1-(tetrazol-5-yl-diazenyl)guanidin monohydrate, 1-guanyl-4-nitrosoaminoguanyltetrazene, tetracene (older lit.), guanyldiazoguanyl tetrazene [tetrazen, GNGT]

Main (potential) use: Primary explosive, used in detonators if initiated by another primary explosive^[4], often used to sensitize other primary explosives^[12], intermediate booster in detonators if initiated by another primary explosive or mixed with another primary explosive^[14], priming compositions and with LA in explosive rivets^[18], ingredient of primer and detonator compositions^[19, 20], component of priming compositions or as an intermediate booster^[22], environmentally friendly primary explosive^[25], in impact primers and prick blasting caps as an additive to LA and LS^[25], sensitization of priming compositions^[26]

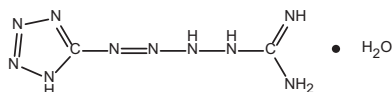
Structural formula:



X-ray structure



Historical formula I



Historical formula II

* Tetrazene forms a hydrate with 3 molecules of water^[4]

	Tetrazene*
Formula	C ₂ H ₈ N ₁₀ O
Molecular mass [g mol ⁻¹]	188.16

Appearance at RT	Colorless, pale yellow crystals (crystallizes as monohydrate) ^[10] , colorless or pale yellow fluffy solid ^[4, 14, 18, 19, 22] , needle crystals ^[4] , pale yellow ^[20]																	
IS [J]	<p>1 Nm^[3], 7 cm (2 kg mass, B.M.)^[4, 6, 20, 22], 8 in (8 ounce mass, P.A.)^[4, 6, 14], 10 cm (2 kg mass)^[8], ~ 0.5^[10], 1.0^[10], 1.4^[10], 0.5 (P.A.)^[10], 1.4 (B.M.)^[10], 2 in (2 kg mass, P.A.)^[22], 0.021^[26], H_{10%} = 8 in (2 kg mass, P.A.)^[28], 17.0 in (ball drop, 7 g ball impacting on a 0.5 mm thick layer of sample)^[28], H_{10%} = 14 in (ball drop test, 8.35 g, ½ in diameter steel ball, 35 mg sample)^[31], H_{50%} = 18 in (ball drop test, 8.35 g, ½ in diameter steel ball, 35 mg sample)^[31], 6.0 cm (100% fire, 400 g hammer, 20 mg sample)^[33], 3.5 cm (100% no-fire, 400 g hammer, 20 mg sample)^[33]</p> <p>No. of positive trials out of 5 @ specific drop-heights^[11]:</p> <table><tr><th>Drop-height (cm)</th><th>No. of detonations out of 5 trials</th></tr><tr><td>16</td><td>2</td></tr><tr><td>19</td><td>2</td></tr><tr><td>17</td><td>3</td></tr><tr><td>20</td><td>3</td></tr><tr><td>23</td><td>3</td></tr><tr><td>24</td><td>4</td></tr></table> <p>Minimum hot-spot <i>T</i> for initiation by impact = 400–430 °C (in the presence of grit)^[16]</p>	Drop-height (cm)	No. of detonations out of 5 trials	16	2	19	2	17	3	20	3	23	3	24	4			
Drop-height (cm)	No. of detonations out of 5 trials																	
16	2																	
19	2																	
17	3																	
20	3																	
23	3																	
24	4																	
FS [N]	<p>8.57^[10], 70% (explosion % of 25 samples under 588.40 kPa and 80° swing angle)^[33]</p> <p>FS (g) tested on porcelain and Emery paper (Julius-Peters BAM)^[13]:</p> <table><tr><th rowspan="2">Porcelain</th><th colspan="5">Emery paper grades</th></tr><tr><th>P80</th><th>P100</th><th>P120</th><th>P180</th><th>P360</th></tr><tr><td>430</td><td>> 2,075</td><td>1,000</td><td>700</td><td>1,000</td><td>> 2,075</td></tr></table> <p><i>F</i>₅₀ = 7.53 (dry sample) (FSKM-PEx OZM friction tester, roughened ceramic plate and porcelain peg)^[17], <i>F</i>₅₀ = 34.55 (5% water) (FSKM-PEx OZM friction tester, roughened ceramic plate and porcelain peg)^[17], <i>F</i>₅₀ = 20.05 (10% water) (FSKM-PEx OZM friction tester, roughened ceramic plate and porcelain peg)^[17], <i>F</i>₅₀ = 30.14 (20% water) (FSKM-PEx OZM friction tester, roughened ceramic plate and porcelain peg)^[17], <i>F</i>₅₀ = 28.56 (excess water) (FSKM-PEx OZM friction tester, roughened ceramic plate and porcelain peg)^[17]</p>	Porcelain	Emery paper grades					P80	P100	P120	P180	P360	430	> 2,075	1,000	700	1,000	> 2,075
Porcelain	Emery paper grades																	
	P80	P100	P120	P180	P360													
430	> 2,075	1,000	700	1,000	> 2,075													

	<p>$F_{50\%} = 850 \pm 350$ g (Julius-Peters, BAM, porcelain plate and peg, Bruceton method, Tetrazene 407913)^[23], $F_{10\%} = 300$ g (Julius-Peters, BAM, porcelain plate and peg, Bruceton method, Tetrazene 407913)^[23], $F_{50\%} = 900 \pm 180$ g (Julius-Peters, BAM, porcelain plate and peg, Bruceton method, Tetrazene 7902454)^[23], $F_{10\%} = 700$ g (Julius-Peters, BAM, porcelain plate and peg, Bruceton method, Tetrazene 7902454)^[23]</p> <p>No fire @ 1,100 g but low fire @ 1,200 g (Julius-Peters, BAM)^[26]</p>																																										
ESD [J]	<p>0.01^[4], 0.010 (unconfined)^[6, 20], 0.012 (confined)^[6, 20], 2.7 mJ^[10], no fire >7.43 mJ^[26], 0.006 (minimum energy)^[28, 33]</p> <p>Highest electrostatic discharge energy @ 5,000 V for zero ignition probability^[7]:</p> <table><tr><th colspan="2">Highest E for zero ignition probability^[7]</th><th colspan="2">Type of ignition^[7]</th></tr><tr><th>Unconfined</th><th>Confined</th><th>Unconfined</th><th>Confined</th></tr><tr><td>0.010</td><td>0.012</td><td>Low order detonation</td><td>Low order detonation</td></tr></table> <p>Approaching-electrode electrostatic sensitivity apparatus^[32]:</p> <table><tr><th rowspan="2">Discharge</th><th colspan="3">Minimum energy (10⁻⁷ J)</th></tr><tr><th>Approaching needle</th><th>Approaching (pin) plane-to-plane</th><th>Fixed-gap, parallel-plate</th></tr><tr><td>Oscillatory</td><td>~ 200,000 (unclear in original report)</td><td>56,000</td><td>18,500</td></tr><tr><td>Arc</td><td>53,000</td><td>26,000</td><td>4,000</td></tr><tr><td rowspan="2">Spark</td><td>20,000</td><td>4,500</td><td>1,300</td></tr><tr><td>50% point</td><td></td><td></td></tr><tr><td>Spark</td><td>62,000</td><td>–</td><td>9,600</td></tr></table> <p>50% initiation values (spark discharge)^[34]:</p> <table><tr><th>Energy (J × 10⁻⁴) parallel plane, fixed gap</th><th>Approaching needle</th></tr><tr><td>>9.6</td><td>62</td></tr></table>	Highest E for zero ignition probability ^[7]		Type of ignition ^[7]		Unconfined	Confined	Unconfined	Confined	0.010	0.012	Low order detonation	Low order detonation	Discharge	Minimum energy (10 ⁻⁷ J)			Approaching needle	Approaching (pin) plane-to-plane	Fixed-gap, parallel-plate	Oscillatory	~ 200,000 (unclear in original report)	56,000	18,500	Arc	53,000	26,000	4,000	Spark	20,000	4,500	1,300	50% point			Spark	62,000	–	9,600	Energy (J × 10 ⁻⁴) parallel plane, fixed gap	Approaching needle	>9.6	62
Highest E for zero ignition probability ^[7]		Type of ignition ^[7]																																									
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Energy (J × 10 ⁻⁴) parallel plane, fixed gap	Approaching needle																																										
>9.6	62																																										
N [%]	74.44																																										
Ω(CO ₂) [%]	–59.5																																										

$T_{m.p.}$ [°C]	<p>140–160 (dec. with explosion)^[4, 19, 20, 22], 142 (dec.)^[6]</p> <p>DSC (T_o = onset T of peak, T_p = peak T of thermal event, ΔH = heat absorbed), tetrazene is melt-dehydrated @ 128.4 °C^[26]:</p> <table><tr><th rowspan="2">Heating rate</th><th colspan="3">Endothermic peaks</th></tr><tr><th>T_o (°C)</th><th>T_p (°C)</th><th>ΔH (J/g)</th></tr><tr><td>2 K/min</td><td>123.0</td><td>128.4</td><td>–50.0</td></tr><tr><td>5 K/min</td><td>127.8</td><td>133.8</td><td>–26.4</td></tr></table>	Heating rate	Endothermic peaks			T_o (°C)	T_p (°C)	ΔH (J/g)	2 K/min	123.0	128.4	–50.0	5 K/min	127.8	133.8	–26.4																																																			
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5 K/min	127.8	133.8	–26.4																																																																
$T_{dec.}$ [°C]	<p>136 (DSC @ 20 °C/min)^[1], 142^[6], ≥ 60 in presence of moisture^[10], explodes @ 408 K if heated slowly in vacuum, whereas rapid heating to 440 K only causes rapid volatilization of the products, no melting was observed (Yoffe)^[12], ~ 140 (onset of intense dec.)^[25], 138 (onset), 144 (peak) (DSC @ 20 °C/min)^[26]</p> <p>Mass loss data from nonisothermal TG curves (T_i = initial T for thermal dec.; T_{ot} = onset T for dec.; L_{max} = max mass loss rate; T_p = peak T of mass loss rate, T_{oe} = end T of DTG peak)^[26]:</p> <table><tr><th colspan="4">TG curves</th><th colspan="3">DTG peaks</th></tr><tr><th>β (°C/min)</th><th>T_i (°C)</th><th>T_{ot} (°C)</th><th>Mass loss (%)</th><th>L_{max} (%/min)</th><th>T_p (°C)</th><th>T_{oe} (°C)</th></tr><tr><td>1.0</td><td>118.6</td><td>112.5</td><td>–19.7</td><td>–3.03</td><td>126.3</td><td>131.7</td></tr><tr><td>2.0</td><td>124.8</td><td>113.7</td><td>–20.5</td><td>–5.23</td><td>131.2</td><td>137.0</td></tr><tr><td>3.0</td><td>129.8</td><td>116.2</td><td>–19.3</td><td>–8.73</td><td>134.9</td><td>139.9</td></tr><tr><td>4.0</td><td>133.1</td><td>124.6</td><td>–20.3</td><td>–15.48</td><td>137.8</td><td>142.0</td></tr></table> <p>DSC (T_{ot} = onset T of peak, T_p = peak T of thermal event, ΔH = heat released, T_{sp} = shoulder peak, T_e = end T for heat change)^[26]:</p> <table><tr><th rowspan="2"></th><th colspan="4">Exothermic peaks</th></tr><tr><th>T_o (°C)</th><th>T_p; T_{sp} (°C)</th><th>T_e (°C)</th><th>ΔH (J/g)</th></tr><tr><td>2 K/min</td><td>131.7</td><td>133.1; 158.2</td><td>136.4</td><td>1,037</td></tr><tr><td>5 K/min</td><td>138.5</td><td>140.9; 168.9</td><td>142.5</td><td>905</td></tr><tr><td>5 °C/min (cited in^[26])</td><td></td><td>140.5; 167.6</td><td></td><td>590 ± 20</td></tr></table>	TG curves				DTG peaks			β (°C/min)	T_i (°C)	T_{ot} (°C)	Mass loss (%)	L_{max} (%/min)	T_p (°C)	T_{oe} (°C)	1.0	118.6	112.5	–19.7	–3.03	126.3	131.7	2.0	124.8	113.7	–20.5	–5.23	131.2	137.0	3.0	129.8	116.2	–19.3	–8.73	134.9	139.9	4.0	133.1	124.6	–20.3	–15.48	137.8	142.0		Exothermic peaks				T_o (°C)	T_p ; T_{sp} (°C)	T_e (°C)	ΔH (J/g)	2 K/min	131.7	133.1; 158.2	136.4	1,037	5 K/min	138.5	140.9; 168.9	142.5	905	5 °C/min (cited in ^[26])		140.5; 167.6		590 ± 20
TG curves				DTG peaks																																																															
β (°C/min)	T_i (°C)	T_{ot} (°C)	Mass loss (%)	L_{max} (%/min)	T_p (°C)	T_{oe} (°C)																																																													
1.0	118.6	112.5	–19.7	–3.03	126.3	131.7																																																													
2.0	124.8	113.7	–20.5	–5.23	131.2	137.0																																																													
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5 K/min	138.5	140.9; 168.9	142.5	905																																																															
5 °C/min (cited in ^[26])		140.5; 167.6		590 ± 20																																																															

ρ [g cm ⁻³]	1.7 (@ 293 K) ^[3] , 1.7 (crystal @ 20 °C) ^[4] , 0.45 (apparent ρ) ^[4, 6, 14] , 1.05 (pellet, if compressed @ 3,000 psi) ^[6, 20] , 0.5 (apparent ρ) ^[8] , 1.64–1.65 (crystal) ^[10] , 0.45 (bulk) ^[10] , 1.05 (when compressed under 3,000 lb/in ²) ^[4, 14] , 1.7 (crystal) ^[4, 23] , 1.63 (crystal) ^[25] Loading ρ @ different pressures ^[9] : <table><tr><th>Pressure (kpsi)</th><th>Loading ρ (g cm⁻³)</th></tr><tr><td>3</td><td>1.05^[9, 24]</td></tr><tr><td>5</td><td>1.22^[9, 24]</td></tr><tr><td>10</td><td>1.33^[9, 24]</td></tr><tr><td>12</td><td>1.37^[9, 24]</td></tr><tr><td>15</td><td>1.41^[9, 24]</td></tr><tr><td>20</td><td>1.48^[9, 24]</td></tr><tr><td>Crystal</td><td>1.72^[9]</td></tr></table>			Pressure (kpsi)	Loading ρ (g cm ⁻³)	3	1.05 ^[9, 24]	5	1.22 ^[9, 24]	10	1.33 ^[9, 24]	12	1.37 ^[9, 24]	15	1.41 ^[9, 24]	20	1.48 ^[9, 24]	Crystal	1.72 ^[9]
Pressure (kpsi)	Loading ρ (g cm ⁻³)																		
3	1.05 ^[9, 24]																		
5	1.22 ^[9, 24]																		
10	1.33 ^[9, 24]																		
12	1.37 ^[9, 24]																		
15	1.41 ^[9, 24]																		
20	1.48 ^[9, 24]																		
Crystal	1.72 ^[9]																		
Heat of formation	212 kJ/mol (heat of form., ΔH_f) ^[2] , 1,005 kJ/kg (enthalpy of form.) ^[3] , 270 g cal/mol ^[4]																		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.																
$-\Delta_{\text{ex}}U^\circ$ [kJ kg ⁻¹]	2,623		2,755 ^[2] 658 cal/g ^[4, 6, 20]																
T_{ex} [K]	2,002																		
$p_{\text{C-J}}$ [kbar]	26.8																		
VoD [m s ⁻¹]	8,820 (@ TMD)																		
V_0 [L kg ⁻¹]	922	1,190 cc/g ^[6]	1,190 cm ³ /g ^[4, 20]																
Trauzl test [cm ³ , % TNT]	51–63% TNT ^[4] , 61% TNT ^[6, 20, 22]																		
Sand test [g]	28.0 g sand crushed (cf. 48.0 g TNT) by 0.4 g Tetrazene initiated by No. 6 cap ^[4] , 40–70% TNT ^[4] , max. brisance = 21.2 g sand crushed by 0.4 g Tetracene compressed @ 3,000 lb/in ² initiated by fulminate ^[4, 14] , 22.6 g sand crushed by 0.4 g Tetracene using compound primer of 0.15 g Tetryl initiated with 0.25 g mercury fulminate ^[14] , 13.1 g (loose Tetrazene) ^[4] , 2 g (if Tetrazene loaded under pressure of 3,000 lb/in ²) ^[4] , 28.0 g (200 g bomb) ^[22]																		

	Values from ^[14] : <table><tr><td>Amount of Tetracene (g)</td><td>Compressed under pressure (lb/in²)</td><td>Amount of sand crushed (g)</td></tr><tr><td>0.4</td><td>Not compressed</td><td>13.1</td></tr><tr><td>0.4</td><td>Compressed @ 250</td><td>9.2</td></tr><tr><td>0.4</td><td>Compressed @ 500</td><td>7.5</td></tr><tr><td>0.4</td><td>Compressed @ 3,000</td><td>2.0</td></tr></table>	Amount of Tetracene (g)	Compressed under pressure (lb/in ²)	Amount of sand crushed (g)	0.4	Not compressed	13.1	0.4	Compressed @ 250	9.2	0.4	Compressed @ 500	7.5	0.4	Compressed @ 3,000	2.0									
Amount of Tetracene (g)	Compressed under pressure (lb/in ²)	Amount of sand crushed (g)																							
0.4	Not compressed	13.1																							
0.4	Compressed @ 250	9.2																							
0.4	Compressed @ 500	7.5																							
0.4	Compressed @ 3,000	2.0																							
Initiating efficiency	<p>0.40 g MF minimum detonating charge^[4, 20]</p> <p>Minimum charges necessary to initiate PETN (0.4 g PETN tamped down or loosely pressed into Cu capsules, 6.2 mm inside diameter, primary charge placed loosely on top, values given for min. weight or primary charge that shows one failure; or 0.4 g PETN compressed @ 2,000 kg/cm², priming charges either loosely placed on top or pressed on top of compressed PETN @ 500, 1,000 or 1,500 kg/cm²)^[14]:</p> <table><tr><td>Pressure on PETN (kg/cm²)</td><td>0</td><td>2,000</td><td>2,000</td><td>2,000</td><td>2,000</td></tr><tr><td>Pressure on initiator (kg/cm²)</td><td>0</td><td>0</td><td>500</td><td>1,000</td><td>1,500</td></tr><tr><td>Primary explosive</td><td colspan="5">Minimum initiating charge (g)</td></tr><tr><td>Tetracene</td><td>0.16</td><td>0.250</td><td colspan="3">Dead-pressed</td></tr></table> <p>Pressed tetrazene does not detonate PETN^[19], does not detonate TNT^[22], only detonates PETN and Tetryl if the tetrazene is unpressed^[22], minimum charge of 0.25 g in No. 8 detonator required for PETN^[25]</p>	Pressure on PETN (kg/cm ²)	0	2,000	2,000	2,000	2,000	Pressure on initiator (kg/cm ²)	0	0	500	1,000	1,500	Primary explosive	Minimum initiating charge (g)					Tetracene	0.16	0.250	Dead-pressed		
Pressure on PETN (kg/cm ²)	0	2,000	2,000	2,000	2,000																				
Pressure on initiator (kg/cm ²)	0	0	500	1,000	1,500																				
Primary explosive	Minimum initiating charge (g)																								
Tetracene	0.16	0.250	Dead-pressed																						
Dead-pressing	Easily dead-pressed ^[4, 14] , extremely sensitive to dead-pressing ^[19] , loses ability in No. 8 blasting cap to initiate on being compressed at pressures >15 MPa ^[25]																								
5 s explosion <i>T</i> [°C] Explosion <i>T</i> [°C] Ignition <i>T</i> [°C] Autoignition <i>T</i> [K] Thermal ignition <i>T</i> [°C]	160 ^[4, 6, 14, 20, 22, 24, 33] 140 ^[8] , explodes in the solid state in the <i>T</i> range 408–418 K ^[12] , 150 ^[19] , explodes @ 408 K if heated slowly in vacuum, whereas rapid heating to 440 K only causes rapid volatilization of the products, no melting was observed (Yoffe) ^[12] , 154 ^[18] 160 ^[16] , ~ 160 ^[25] , 147 ^[30] 395 (Tetrazene 407913) ^[23] , 393 (Tetrazene 7902454) ^[23] 160 (calcd.) ^[24]																								

Thermal stability

Relatively stable @ $T < 75\text{ }^{\circ}\text{C}$ ^[4, 19], stable @ RT wet or dry^[14], dec. by boiling H_2O ^[14], no significant change in power if stored at moderately elevated T ^[18], stable at $T < 75\text{ }^{\circ}\text{C}$, but dec. at higher T with dec. rate increasing rapidly as T increases^[22], slow dec. @ $60\text{ }^{\circ}\text{C}$ and complete dec. @ $90\text{ }^{\circ}\text{C}$ after 6 days^[25], low thermal stability with complete dec. @ $90\text{ }^{\circ}\text{C}$ in 6 days^[26], complete dec. in boiling water^[26], 36.1% weight loss @ 167 h (TGA)^[26], deteriorated in 5 weeks @ $60\text{ }^{\circ}\text{C}$ or 8 days @ $75\text{ }^{\circ}\text{C}$ or 3 h @ $100\text{ }^{\circ}\text{C}$ (commercial sample)^[29], deteriorated in >13 weeks @ $60\text{ }^{\circ}\text{C}$ or 14 days @ $75\text{ }^{\circ}\text{C}$ or 7.5 h @ $100\text{ }^{\circ}\text{C}$ (commercial sample)^[29], dec. too slow @ $60\text{ }^{\circ}\text{C}$ for short-term expts.^[29], withstands $75\text{--}80\text{ }^{\circ}\text{C}$ for short periods^[29], dec. complete within 1 week @ $90\text{ }^{\circ}\text{C}$ ^[29], recovered unchanged after 91 days @ $65\text{ }^{\circ}\text{C}$ ^[29], @ $89\text{ }^{\circ}\text{C}$ after 6 weeks 20% Tetrazene sample remains and 50% mass loss occurs^[29], 3% of residual sample remains after 5 weeks @ $89\text{ }^{\circ}\text{C}$ (large sample)^[29]

Analysis results^a for Tetrazene samples undergoing thermal degradation at $89\text{ }^{\circ}\text{C}$ (^a = all measurements were made in duplicate and represent mean values; ^b = samples weighed directly into DSC pans and stored at $89\text{ }^{\circ}\text{C}$; ^c = sample originally 1.25 g, stored in covered petric dish at $89\text{ }^{\circ}\text{C}$; ^d = as a percent of the total original mass. Numbers in parenthesis are percent in remaining mass to afford a direct comparison with results for large sample; ^e = as a percent of the total mass of sample removed for analysis. This does not take into account mass losses by volatilization of decomposition products; ^f = very broad, difficult to measure T_{max})^[29]:

Time elapsed (days)	Small samples ^b			Large sample ^c	
	Mass loss (%) of total)	Residual tetrazene content (%) ^d	Thermo-gram T_{max} ($^{\circ}\text{C}$)	Residual tetrazene content (%) ^e	Thermo-gram T_{max} ($^{\circ}\text{C}$)
0	0.0	100.0 (100.0)		100.0	
1	0.6	95.6 (95.7)	149.9	95.7	150.4
4	2.6	82.7 (84.6)	148.8	90.1	149.1
7	5.0	71.7 (77.4)	148.1	80.5	148.2
10	10.4	62.3 (72.3)	148.4	60.4	148.6
14	19.5	55.1 (67.1)	148.8	45.6	148.1
18	24.5	41.6 (54.7)	148.7	32.9	148.7
21	27.5	44.9 (60.9)	148.7	32.7	148.2
28	35.1	33.8 (51.3)	148.3	13.0	147.5 ^f
35	42.7	17.1 (29.7)	148.5	~ 3	~ 146 ^f
42	46.9	20.0 (36.5)	149.6	< 3	~ 147 ^f

Flame sensitivity	1,000 MPa compacting pressure, 1 mm orifice diameter ^[11] :										
	<table><tr><td>Time in hydrogen/air flame (ms)</td><td>Prob. of initiation (%)</td></tr><tr><td>~2.4</td><td>0</td></tr><tr><td>~2.6</td><td>~ 16</td></tr><tr><td>~3.2</td><td>~ 56</td></tr><tr><td>~6.5</td><td>100</td></tr></table>	Time in hydrogen/air flame (ms)	Prob. of initiation (%)	~2.4	0	~2.6	~ 16	~3.2	~ 56	~6.5	100
	Time in hydrogen/air flame (ms)	Prob. of initiation (%)									
	~2.4	0									
	~2.6	~ 16									
	~3.2	~ 56									
~6.5	100										
0 MPa compacting pressure, 3 mm orifice diameter ^[11] :											
<table><tr><td>Time in hydrogen/air flame (ms)</td><td>Prob. of initiation (%)</td></tr><tr><td>1.5</td><td>0</td></tr><tr><td>~1.4</td><td>20</td></tr><tr><td>~1.5</td><td>50</td></tr><tr><td>~1.6</td><td>100</td></tr></table>	Time in hydrogen/air flame (ms)	Prob. of initiation (%)	1.5	0	~1.4	20	~1.5	50	~1.6	100	
Time in hydrogen/air flame (ms)	Prob. of initiation (%)										
1.5	0										
~1.4	20										
~1.5	50										
~1.6	100										
Undergoes mild explosion producing a lot of black smoke on contact with flame ^[4, 19] , detonates readily on exposure to flame ^[22]											
Specific heat [J kg ⁻¹ K ⁻¹ × 10 ²]	15.85 ± 0.65 (temperature range 290–400 K) ^[12] , 16.3 (lit. value) ^[12]										
Activation energy for dec. [kJ/mol]	148 (Tetracene A, slow dec. studies, <i>Bird</i>) ^[12] , 138 (Tetrazene B, slow dec. studies, <i>Bird</i>) ^[12] , 360 (<i>Krien</i>) ^[12]										
100 °C heat test [% mass loss]	Extreme dec. in first 48 h ^[4] , 23.2% mass loss in first 48 h ^[6, 20] , 3.4% in second 48 h ^[6, 20] , no explosion in 100 h ^[6, 20]										
International test @ 75 °C	0.5% mass loss in 48 h ^[4, 6, 20]										
Burn rate [mm/s]	Undergoes mild explosion producing black smoke on contact with flame ^[19]										
Solubility [g/mL]	Practically insoluble in H ₂ O and most organic solvents, e.g. EtOH, acetone, Et ₂ O, benzene ^[10] , practically insoluble in H ₂ O, EtOH, Et ₂ O, benzene, CCl ₄ ^[4, 14, 19, 20] , practically insoluble in acetone and ethylene dichloride ^[4] , soluble in dil. nitric acid or strong hydrochloric acid ^[4]										
Hygroscopicity	Slightly hygroscopic ^[10, 14, 22] , absorbs 0.77% H ₂ O @ 30 °C, 90% rel. humidity ^[4, 10, 20] , hydrolytically unstable ^[26]										
Compatibility	Does not react with conc. HNO ₃ , steel, Cu, Al, TNT, Tetryl, PETN, or RDX @ RT ^[10] , dec. by boiling H ₂ O ^[4, 14, 20] , reacts with excess of AgNO ₃ ^[4] , dec. by wet CO ₂ ^[25] , hydrolytically stable: DSC showed >99% sample purity after 2 months suspended in water @ 20 °C ^[29]										

Blast characteristics	<p>Values from^[15] (loose-filled into mild steel test units (4.6 × 2.5 × 2.5 cm), 0.9 cm hole diameter, sealed with cork disc and adhesive, mass of material = 200–1,000 g, initiated with ICI type “E” fuzehead):</p> <table><tr><th>Material</th><th>Blast wave peak overpressure, P_{\max} (kPa) (mean value)</th><th>Blast wave positive phase impulse I^* (Pa s) (mean value)</th></tr><tr><td>Tetracene</td><td>3.2</td><td>0.32</td></tr><tr><td>Tetracene/Na_2CO_3 (90:10) (proportions by weight)</td><td>2.8</td><td>0.24</td></tr><tr><td>Tetracene/NaNO_2 (90:10) (proportions by weight)</td><td>2.8</td><td>0.23</td></tr></table> <p>TNT equivalence = 0.42 (average between scaled distances 10 $\text{mkg}^{-1/3}$ and 25 $\text{mkg}^{-1/3}$)^[15]</p>	Material	Blast wave peak overpressure, P_{\max} (kPa) (mean value)	Blast wave positive phase impulse I^* (Pa s) (mean value)	Tetracene	3.2	0.32	Tetracene/ Na_2CO_3 (90:10) (proportions by weight)	2.8	0.24	Tetracene/ NaNO_2 (90:10) (proportions by weight)	2.8	0.23						
Material	Blast wave peak overpressure, P_{\max} (kPa) (mean value)	Blast wave positive phase impulse I^* (Pa s) (mean value)																	
Tetracene	3.2	0.32																	
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Tetracene/ NaNO_2 (90:10) (proportions by weight)	2.8	0.23																	
Stab sensitivity	<p>Stab initiation energies for admixtures of lead azide with tetrazene which had been subjected to thermal and hydrolytic stability studies (Tetrazene/LA RD1343 (1:20 by weight), compacted @ 560 MPa into stab detonator)^[29]:</p> <table><tr><th>Test/time elapsed</th><th>Stab initiation energies (mj)</th></tr><tr><td colspan="2">thermal stability at 89 °C</td></tr><tr><td>0</td><td>3.6</td></tr><tr><td>1 week</td><td>3.9</td></tr><tr><td>2 weeks</td><td>6.6</td></tr><tr><td>3 weeks</td><td>6.9</td></tr><tr><td>4 weeks</td><td>10.2</td></tr><tr><td>5 weeks</td><td>20</td></tr><tr><td>6 weeks</td><td>110</td></tr></table>	Test/time elapsed	Stab initiation energies (mj)	thermal stability at 89 °C		0	3.6	1 week	3.9	2 weeks	6.6	3 weeks	6.9	4 weeks	10.2	5 weeks	20	6 weeks	110
Test/time elapsed	Stab initiation energies (mj)																		
thermal stability at 89 °C																			
0	3.6																		
1 week	3.9																		
2 weeks	6.6																		
3 weeks	6.9																		
4 weeks	10.2																		
5 weeks	20																		
6 weeks	110																		
Ignition sensitivity by electric bridge current	<p>Bridge current and ignition time (I = ignition current (ampere), s = ignition time (1/1,000 s), I^2s = (ignition current)² × (ignition time))^[30]:</p> <table><tr><td>I</td><td>2.0</td><td>1.6</td><td>1.3</td><td>1.0</td><td>0.8</td></tr><tr><td>s</td><td>2.4</td><td>3.1</td><td>4.1</td><td>5.3</td><td>6.6</td></tr><tr><td>I^2s</td><td>9.6</td><td>7.9</td><td>6.9</td><td>5.3</td><td>4.2</td></tr></table>	I	2.0	1.6	1.3	1.0	0.8	s	2.4	3.1	4.1	5.3	6.6	I^2s	9.6	7.9	6.9	5.3	4.2
I	2.0	1.6	1.3	1.0	0.8														
s	2.4	3.1	4.1	5.3	6.6														
I^2s	9.6	7.9	6.9	5.3	4.2														
Brisance	40–70% TNT ^[4]																		

	Tetrazene ^[5]	Tetrazene ^[5]
Chemical formula	C ₂ H ₈ N ₁₀ O	C ₂ H ₈ N ₁₀ O
Molecular weight [g mol ⁻¹]	188.16	188.16
Crystal system	Monoclinic	Monoclinic
Space group	<i>Ia</i>	<i>P 2₁/ a</i>
<i>a</i> [Å]	12.888(1)	12.955(2)
<i>b</i> [Å]	9.332(1)	9.295(1)
<i>c</i> [Å]	6.811(1)	6.847(1)
α [°]	90	90
β [°]	112.47(1)	111.54(1)
γ [°]	90	90
<i>V</i> [Å ³]	756.973	766.912
<i>Z</i>	Not given	4
ρ_{calc} [g cm ⁻³]	Not given	1.63
<i>T</i> [K]	295	295

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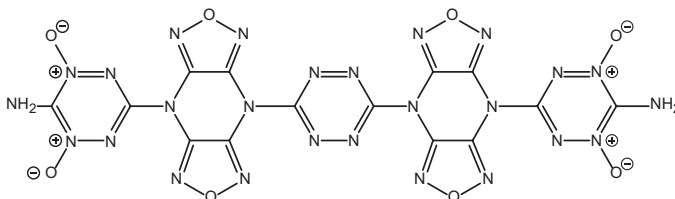
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6,6'-{1,2,4,5-Tetrazine-3,6-diylbis[(4*H*,8*H*-bis[1,2,5]oxadiazolo[3,4-*b*:3',4'-*e*]pyrazine-8,4-diyl)]}bis(2,4-dioxo-1,2,4,5-tetrazin-3-amine)

Name [German, acronym]: 3,3'-((1,4-Dioxido-1,2,4,5-tetrazine-3,6-diyl)bis(4*H*,8*H*-bis[1,2,5]oxadiazolo[3,4-*b*:3',4'-*e*]pyrazine-8,4-diyl))bis(6-amino-1,2,4,5-tetrazine 1,5-dioxide)

Main (potential) use: thermally stable explosive

Structural formula:



Formula	C ₁₄ H ₄ N ₂₆ O ₈		
Molecular mass [g mol ⁻¹]	664.36		
Appearance at RT	Clear block orange crystals (solvate with DMF) ^[1]		
IS [J]	<i>H</i> _{50%} = 35.7 (LANL type 12, 2.5 kg mass) ^[1]		
FS [N]	>360 (50% load, Bruceton up/down method) ^[1]		
ESD [J]	0.062 (ABL spark, 3.4% threshold initiation level) ^[1]		
<i>N</i> [%]	54.82		
Ω(CO ₂) [%]	−52.98		
<i>T</i> _{dec.} [°C]	226 (exo, onset), 295 (exo, peak max) (DSC @ 10 °C/min, hermetically sealed Al pan) ^[1]		
<i>ρ</i> [g cm ⁻³]	1.903 (calcd. @ 23 °C) ^[1] , 1.541 (DMF solvate, X-ray @ 296 K) ^[1]		
Heat of formation	2,128 kJ/mol (enthalpy of form., calcd.) ^[1]		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
−Δ _{ex} <i>U</i> ^o [kJ kg ⁻¹]			
<i>T</i> _{ex} [K]			

$p_{C,j}$ [kbar]		32 GPa (@ 1.903 g cm ⁻³ , calcd., CHEETAH) ^[1]	
VoD [m s ⁻¹]		8,700 (@ 1.903 g cm ⁻³ , calcd., CHEETAH) ^[1]	
V_0 [L kg ⁻¹]			
ΔH_{dec} [J/g]	1,211 (DSC @ 10 °C/min, hermetically sealed Al pan) ^[1]		

	6,6'-{1,2,4,5-Tetrazine-3,6-bis[1,2,5]oxadiazolo[3,4-<i>b</i>:3',4'-<i>e</i>]pyrazine-8,4-diyl}}bis(2,4-dioxo-1,2,4,5-tetrazin-3-amine) <i>N,N</i>-dimethylformamide solvate^[1]
Chemical formula	C ₁₄ H ₄ N ₂₆ O ₈ •4DMF
Molecular weight [g mol ⁻¹]	956.81
Crystal system	Triclinic
Space group	<i>P</i> -1 (no. 2)
<i>a</i> [Å]	9.5919(4)
<i>b</i> [Å]	12.8830(6)
<i>c</i> [Å]	17.5266(8)
α [°]	100.2430(10)
β [°]	96.5340(10)
γ [°]	101.589(2)
<i>V</i> [Å ³]	2,062.57(16)
<i>Z</i>	2
ρ_{calc} [g cm ⁻³]	1.541
<i>T</i> [K]	296

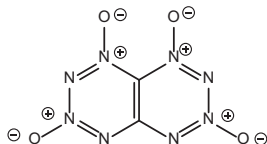
- [1] C. J. Snyder, L. A. Wells, D. E. Chavez, G. H. Imler, D. A. Parrish, *Chem. Comm.*, **2019**, 55, 2461–2464.

Tetrazino-tetrazine-1,3,6,8-tetroxide

Name [German, acronym]: [1,2,3,4]Tetrazino[5,6-e][1,2,3,4]tetrazine
1,3,6,8-tetraoxide, di-tetrazine-tetroxide [TTTO, DTTTO]

Main (potential) use: Possible component of future high-power explosive compositions and solid high propellants^[3]

Structural formula:



	TTTO
Formula	$C_2N_8O_4$
Molecular mass [g mol ⁻¹]	200.07
Appearance at RT	Yellow powder ^[1] , yellow crystals (crude product) ^[3]
IS [J]	~27 (est., 2.5 kg mass, ~ 110 cm, calcd.) ^[5]
FS [N]	No detonation on rubbing in an agate mortar ^[1] , exploded on rubbing in an unglazed porcelain mortar ^[1]
N [%]	56.01
Ω(CO ₂) [%]	0
T _{m,p.} [°C]	183–186 (dec.) ^[1, 3]
T _{b,p.} [°C]	653 K (est., COSMO-RS) ^[7]
T _{dec.} [°C]	183–186 (dec.) ^[1]
ρ [g cm ⁻³]	1.98 (calcd.) ^[1] , 1.96 (calcd., most stable calcd. isomer C ₁ with P2 ₁ 2 ₁ 2 ₁ space group and Z = 4) ^[4] , 1.899 (calcd.) ^[5]
Heat of formation	~206 kcal/mol (calcd.) ^[1] , ΔH _f [°] = 1,030 kcal/kg (calcd.) ^[3] , ΔH _f [°] (g) = 223.3 kcal/mol (calcd., B3LYP) ^[5] , ΔH _f [°] (liq.) = 209.1 kcal/mol (calcd.) ^[5] , ΔH _f [°] (s) = 205.5 kcal/mol (calcd.) ^[5] , ΔH _f [°] = 207.53 kcal/mol (calcd.) ^[6] , 868.3 kJ/mol (enthalpy of form.) ^[7] , 965.9 kJ/mol (ΔH _f (298 K), calcd., W1U) ^[7]

	calcd. gas phase (0 K and 298 K) and liquid (298 K) heats of formation (kJ/mol) ^[7] :																																									
	<table><tr><th>Property</th><th>Method</th><th>DTTO</th></tr><tr><td>ΔH_f (0 K)</td><td>G3MP2</td><td>1,022.4</td></tr><tr><td>ΔH_f (298 K)</td><td>G3MP2</td><td>996.0</td></tr><tr><td>ΔH_f (298 K, liq.)</td><td>G3MP2</td><td>927.4</td></tr><tr><td>ΔH_f (0 K)</td><td>G3</td><td>1,001.1</td></tr><tr><td>ΔH_f (298 K)</td><td>G3</td><td>974.7</td></tr><tr><td>ΔH_f (298 K, liq.)</td><td>G3</td><td>906.0</td></tr><tr><td>ΔH_f (0 K)</td><td>G4MP2</td><td>994.4</td></tr><tr><td>ΔH_f (298 K)</td><td>G4MP2</td><td>968.0</td></tr><tr><td>ΔH_f (298 K, liq.)</td><td>G4MP2</td><td>899.7</td></tr><tr><td>ΔH_f (0 K)</td><td>G4</td><td>975.5</td></tr><tr><td>ΔH_f (298 K)</td><td>G4</td><td>949.1</td></tr><tr><td>ΔH_f (298 K, liq.)</td><td>G4</td><td>880.9</td></tr></table>			Property	Method	DTTO	ΔH_f (0 K)	G3MP2	1,022.4	ΔH_f (298 K)	G3MP2	996.0	ΔH_f (298 K, liq.)	G3MP2	927.4	ΔH_f (0 K)	G3	1,001.1	ΔH_f (298 K)	G3	974.7	ΔH_f (298 K, liq.)	G3	906.0	ΔH_f (0 K)	G4MP2	994.4	ΔH_f (298 K)	G4MP2	968.0	ΔH_f (298 K, liq.)	G4MP2	899.7	ΔH_f (0 K)	G4	975.5	ΔH_f (298 K)	G4	949.1	ΔH_f (298 K, liq.)	G4	880.9
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	234.4 kcal/mol (ΔH_f (g) ^o , calcd., ccCA-P) ^[8] , 230.0 kcal/mol (ΔH_f (g) ^o , calcd., ccCA-S3) ^[8] , 232.2 kcal/mol (ΔH_f (g) ^o , calcd., ccCA-PS3) ^[8] , 233.0 kcal/mol (ΔH_f (g) ^o , calcd., G3) ^[8]																																									
	Calcd. (EXPLO5 V6.05.02)	Lit. values	Exptl.																																							
$-\Delta_{\text{ex}}U^o$ [kJ kg ⁻¹]	4,972 (@ 1.96 g cm ⁻³ , ΔH_f = 206 kcal/mol)	1,967 kcal/kg ^[3] $\Delta H_{\text{det}} = -393.6$ kcal/mol (calcd.) $Q = 1,967$ cal/g ^[5] $Q = 1.978$ kcal/g (calcd.) ^[6]																																								
T_{ex} [K]	3,921 (@ 1.96 g cm ⁻³ , ΔH_f = 206 kJ/mol)																																									

p_{C-1} [kbar]	368 (@ 1.96 g cm ⁻³ , ΔH_f = 206 kJ/mol)	43.2 GPa ^[3] 43.0 GPa (calcd. for most stable calcd. isomer C_1 with $P2_12_12_1$ space group and $Z = 4$, $\rho = 1.96$ g cm ⁻³) ^[4] 432 (@ 1.899 g cm ⁻³ , calcd.) ^[5] calculated values using Cheetah 7.0, assuming enthalpy of formation of 868.3 kJ/mol ^[7] : <table><tr><th>Crystal ρ (g/cm³)</th><th>Detonation pressure (GPa)</th></tr><tr><td>1.80</td><td>37.524</td></tr><tr><td>1.85</td><td>40.310</td></tr><tr><td>1.90</td><td>43.377</td></tr><tr><td>1.95</td><td>46.771</td></tr><tr><td>2.00</td><td>50.529</td></tr><tr><td>2.05</td><td>54.654</td></tr><tr><td>2.10</td><td>59.112</td></tr><tr><td>2.15</td><td>63.876</td></tr><tr><td>2.20</td><td>68.978</td></tr><tr><td>2.25</td><td>74.518</td></tr><tr><td>2.30</td><td>80.598</td></tr><tr><td>2.35</td><td>87.228</td></tr><tr><td>2.40</td><td>94.274</td></tr><tr><td>2.419</td><td>97.018</td></tr><tr><td>2.45</td><td>124.592</td></tr></table>	Crystal ρ (g/cm ³)	Detonation pressure (GPa)	1.80	37.524	1.85	40.310	1.90	43.377	1.95	46.771	2.00	50.529	2.05	54.654	2.10	59.112	2.15	63.876	2.20	68.978	2.25	74.518	2.30	80.598	2.35	87.228	2.40	94.274	2.419	97.018	2.45	124.592	
Crystal ρ (g/cm ³)	Detonation pressure (GPa)																																		
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VoD [m s ⁻¹]	9,287 (@ 1.96 g cm ⁻³ , ΔH_f = 206 kJ/mol)	9,710 (@ 1.98 g cm ⁻³ , calcd.) ^[2] 9,700 (calcd. for most stable calcd. isomer C_1 with $P2_12_12_1$ space group and $Z = 4$, $\rho = 1.96$ g cm ⁻³) ^[4] 9,710 (@ 1.899 g cm ⁻³ , calcd.) ^[5]																																	

		calculated values using Cheetah 7.0, assuming enthalpy of formation of 868.3 kJ/mol ^[7] : <table><tr><th>Crystal ρ (g/cm³)</th><th>VoD (km/s)</th></tr><tr><td>1.80</td><td>8.947</td></tr><tr><td>1.85</td><td>9.130</td></tr><tr><td>1.90</td><td>9.312</td></tr><tr><td>1.95</td><td>9.492</td></tr><tr><td>2.00</td><td>9.669</td></tr><tr><td>2.05</td><td>9.843</td></tr><tr><td>2.10</td><td>10.012</td></tr><tr><td>2.15</td><td>10.176</td></tr><tr><td>2.20</td><td>10.336</td></tr><tr><td>2.25</td><td>10.490</td></tr><tr><td>2.30</td><td>10.637</td></tr><tr><td>2.35</td><td>10.775</td></tr><tr><td>2.40</td><td>10.902</td></tr><tr><td>2.419</td><td>10.947</td></tr><tr><td>2.45</td><td>10.929</td></tr></table>	Crystal ρ (g/cm ³)	VoD (km/s)	1.80	8.947	1.85	9.130	1.90	9.312	1.95	9.492	2.00	9.669	2.05	9.843	2.10	10.012	2.15	10.176	2.20	10.336	2.25	10.490	2.30	10.637	2.35	10.775	2.40	10.902	2.419	10.947	2.45	10.929	
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V_0 [L kg ⁻¹]	736 (@ 1.96 g cm ⁻³ , $\Delta H_f = 206$ kJ/mol)																																		
I_{sp} [Ns g ⁻¹]	2.90 (ISPBKW code) ^[6] , 2.91 (0.48%) (calcd., emp.) ^[6] , 2.77 (−4.49%) (calcd., emp.) ^[6]																																		
Hygroscopicity	TTTO and TTTO•benzene can be handled in open air for a short period of time ^[1]																																		
Compatibility	TTTO unchanged after 1 h @ RT in HNO ₃ /H ₂ SO ₄ /Ac ₂ O system ^[1] , hydrolysis complete within 2 h in 50% aq. EtOH @ 20 °C ^[1] , dec. on silica gel 60 ^[1]																																		
ΔH_{vap} [kcal/mol]	14.2 ^[5]																																		
ΔH_{subl} [kcal/mol]	17.8 ^[5]																																		

	TTTO•benzene ^[1]
Chemical formula	C ₈ H ₆ N ₈ O ₄
Molecular weight [g mol ⁻¹]	278.21
Crystal system	Triclinic
Space group	<i>P</i> -1
<i>a</i> [Å]	6.4875(9)
<i>b</i> [Å]	6.7454(10)
<i>c</i> [Å]	13.2696(19)
α [°]	91.743(3)
β [°]	90.868(3)
γ [°]	108.093(3)
<i>V</i> [Å ³]	551.53(4)
<i>Z</i>	2
ρ_{calc} [g cm ⁻³]	1.675
<i>T</i> [K]	120
	Twinned orange crystals obtained by slow evaporation of TTTO in dry benzene (containing 1% v/v trifluoroacetic acid) in vacuum dessicator over P ₄ O ₁₀

Obtained as TTTO•benzene adduct on recryst. from benzene^[1], crystals not obtained from other solvents and powder X-ray diffraction showed disordered molecules^[1]

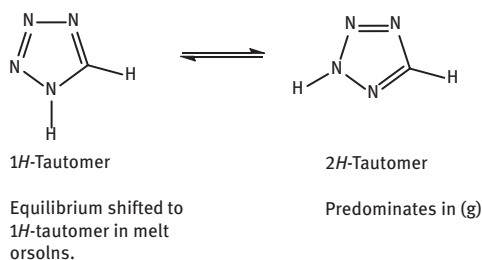
- [1] M. S. Klenov, A. A. Guskov, O. V. Anikin, A. M. Churakov, Y. A. Strelenko, I. V. Fedyanin, K. A. Lyssenko, V. A. Tartakovsky, *Angew. Chem. Int. Ed.*, **2016**, *55*, 11472–11475.
- [2] L. Zhai, F. Bi, Y. Luo, N. Wang, J. Zhang, B. Wang, *Nature Scientific Reports*, **2019**, *9*, Article Nr. 4321.
- [3] M. S. Klenov, A. A. Guskov, O. V. Anikin, A. M. Churakov, V. A. Tartakovskij, *Method for Producing [1,2,3,4]-Tetrazino-[5,6-e]-[1,2,3,4]-Tetrazino-1,3,6,8-Tetraoxide*, Russian Patent RU2, 593,993 C1, 22nd June **2015**.
- [4] C.-C. Ye, Q. An, W. A. Goddard, T. Cheng, W.-G. Liu, S. V. Zybin, X.-H. Ju, *J. Mater. Chem.*, **2015**, *3*, 1972–1978.
- [5] P. Politzer, P. Lane, J. S. Murray, *Centr. Eur. J. Energet. Mater.*, **2013**, *10*, 37–52.
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- [7] K. O. Christe, D. A. Dixon, M. Vasiliev, R. I. Wagner, R. Haiges, J. A. Boatz, H. L. Ammon, *Propellants, Explosives, Pyrotechnics*, **2015**, *40*, 463–468.
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Tetrazole

Name [German, acronym]: α -1*H*-1,2,3,4-Tetrazole* [tetrazol]

Main (potential) use: Precursor for the synthesis of many other energetic materials^[9]

Structural formula:



* Tetrazole can theoretically exist in three tautomeric forms: 1*H*-tetrazole, 2*H*-tetrazole and 5*H*-tetrazole. Both 1*H*-tetrazole and 2*H*-tetrazole have been identified^[11]. In soln. 1*H*- or 2*H*-tetrazole are present, the proportion of tautomers depends on the polarity of the soln. Polar solvents favor the 1*H*-tautomer^[11]

	Tetrazole
Formula	CH ₂ N ₄
Molecular mass [g mol ⁻¹]	70.05
Appearance at RT	Colorless prism crystals ^[4] , crystalline ^[9] , colorless crystals (recryst. from ethyl acetate) ^[10]
IS [J]	<4 (BAM) ^[10] , <4 ^[11]
FS [N]	>360 (none) (BAM) ^[10] , >360 ^[11]
N [%]	79.98
Ω(CO ₂) [%]	-68.52
T _{m.p.} [°C]	156.4 ^[11] , 438 K (broad peak, DSC) ^[4] , 156–157 ^[9] , 154 (endo) (DSC @ 2 °C/min, covered Al pans, N ₂) ^[10] , 155.5 (melts without dec.) ^[5] , 430 ± 1 K (triple-heat-bridge method) ^[12]
T _{phase transition} [°C]	No phase transition observed in DSC ^[4] , 1 <i>H</i> -tautomer exists in crystalline state ^[9] , 1 <i>H</i> - and 2 <i>H</i> -tautomers co-exist in gas-phase with 2 <i>H</i> -tautomer predominating ^[9] , 1 <i>H</i> -tautomer dominates over 2 <i>H</i> -tautomer in polar solvents ^[9] , 1 <i>H</i> -tautomer in melt ^[9] 2 <i>H</i> -tautomer formed during evaporation ^[9]

$T_{\text{dec.}}$ [°C]	188 (exo, dec., DSC @ 2 °C/min, covered Al pans, N ₂) ^[10]														
ρ [g cm ⁻³]	1.632 ^[1] , 1.529 ^[10] , 1.406 (flotation) ^[5] , 1.632 (X-ray) ^[5]														
Heat of formation	<p>237.07 kJ/mol (enthalpy of form.)^[1], 236.0 kJ/mol^[1], 82.3 kcal/mol ($\Delta_f H^\circ_{\text{gas}}$, calcd., G3 method, 1<i>H</i>-tautomer)^[8], 80.4 kcal/mol ($\Delta_f H^\circ_{\text{gas}}$, calcd., G3 method, 2<i>H</i>-tautomer)^[8], 78.3 kcal/mol ($\Delta_f H^\circ_{\text{gas}}$, exptl., 1<i>H</i>-tautomer)^[8], 79.9 kcal/mol ($\Delta_f H^\circ_{\text{gas}}$, exptl., 2<i>H</i>-tautomer)^[8], 78.1 kcal/mol ($\Delta_f H^\circ_{\text{gas}}$, exptl., 1<i>H</i>-tautomer)^[9], 79.1 kcal/mol ($\Delta_f H^\circ_{\text{gas}}$, calcd., W1 level of theory, 1<i>H</i>-tautomer)^[9], 80.2 kcal/mol ($\Delta_f H^\circ_{\text{gas}}$, calcd., CCSD(T)/CBS, 1<i>H</i>-tautomer)^[9], 81.0 kcal/mol ($\Delta_f H^\circ_{\text{gas}}$, calcd., weighted average of G3, G3B3 and CBS-APNO values, 1<i>H</i>-tautomer)^[9], 82.3 kcal/mol ($\Delta_f H^\circ_{\text{gas}}$, calcd., G3, 1<i>H</i>-tautomer)^[9], 77.3 kcal/mol ($\Delta_f H^\circ_{\text{gas}}$, calcd., W1 level of theory, 2<i>H</i>-tautomer)^[9], 79.0 kcal/mol ($\Delta_f H^\circ_{\text{gas}}$, calcd., weighted average of G3, G3B3 and CBS-APNO values, 2<i>H</i>-tautomer)^[9], 80.4 kcal/mol ($\Delta_f H^\circ_{\text{gas}}$, calcd., G3, 2<i>H</i>-tautomer)^[9], 56.66 kcal/mol ($\Delta_f H^\circ_{\text{solid}}$, exptl., static bomb calorimetry, 1<i>H</i>-tautomer)^[9], 79.9 kcal/mol ($\Delta_f H^\circ_{\text{gas}}$, exptl., 1<i>H</i>-tautomer)^[cited in 9], 56.4 kcal/mol ($\Delta_f H^\circ_{\text{solid}}$, exptl., combustion and vapor pressure measurements, 1<i>H</i>-tautomer)^[9], 76.7 kcal/mol ($\Delta_f H^\circ_{\text{gas}}$, exptl., 1<i>H</i>-tautomer)^[9], 78.1 ($\Delta_f H^\circ_{\text{gas}}$, exptl., 1<i>H</i>-tautomer)^[9], 237 kJ/mol ($\Delta H^\circ_{\text{f}}$, calcd.)^[10], 237.224 kJ/mol (enthalpy of form.)^[11] calcd. and exptl. gas phase heats of formation (298 K) in kJ/mol^[13]:</p> <table><tr><td>Method</td><td>1<i>H</i>-Tetrazole</td></tr><tr><td>G3MP2</td><td>346.7</td></tr><tr><td>G3</td><td>344.6</td></tr><tr><td>G4MP2</td><td>333.3</td></tr><tr><td>G4</td><td>330.7</td></tr><tr><td>Exptl.</td><td>334.5 ± 4.2 321.1 ± 2.9 358.8</td></tr></table>			Method	1 <i>H</i> -Tetrazole	G3MP2	346.7	G3	344.6	G4MP2	333.3	G4	330.7	Exptl.	334.5 ± 4.2 321.1 ± 2.9 358.8
Method	1 <i>H</i> -Tetrazole														
G3MP2	346.7														
G3	344.6														
G4MP2	333.3														
G4	330.7														
Exptl.	334.5 ± 4.2 321.1 ± 2.9 358.8														
Heat of combustion	$\Delta U_{\text{comb.}} = -3,281 \text{ cal/g}^{[10]}$, $\Delta H_{\text{comb.}} = -916 \text{ kJ/mol}^{[10]}$														
	Calcd. (EXPLO5 5.02)	Lit. values	Exptl.												
$-\Delta_{\text{ex}} U^\circ$ [kJ kg ⁻¹]	3,941 ^[10]														
T_{ex} [K]	3,047 ^[10]														
$p_{\text{C-J}}$ [kbar]	210 ^[10, 11]														

VoD [m s ⁻¹]	7,813 (@ 1.529 g cm ⁻³) ^[10, 11]												
V ₀ [L kg ⁻¹]	785												
Volatility	Crystals obtained by slow sublimation @ 50 °C ^[5]												
Enthalpy of fusing [kJ/mol]	17.7 ^[1] , Δ _{fus} H ^o _m = 18.0 ± 0.5 kJ/mol (triple-heat-bridge method) ^[12]												
Enthalpy of boiling [kJ/mol]	79.6 ^[1]												
Enthalpy of sublimation [kJ/mol]	97.3 ^[1] , 90.1 ^[1] , 88.0 ^[1] , 125.5 (exptl.) ^[3] , 95.0 (calcd., QSPR) ^[3] , 23.26 kcal/mol (exptl.) ^[9] , 20.2 kcal/mol (exptl.) ^[9] , 21.5 kcal/mol (exptl.) ^[9] , 21.4 kcal/mol (exptl., differential heat-conduction microcalorimetry) ^[9]												
Heat of decomposition [kJ/mol]	162 ^[1] , 216 ^[1]												
Thermal conductivity, λ _c [J/s•cm•K]	0.0125 ^[1]												
Specific heat, C _p [J/g•K]	243 ^[1]												
Surface T (T _s) [°C]	Values from. ^[1] <table><tr><td>P (atm.)</td><td>T_s (°C) (min. and max. measured values)</td></tr><tr><td>1</td><td>250–302</td></tr><tr><td>3.5</td><td>300–422</td></tr><tr><td>8</td><td>368–515</td></tr><tr><td>13</td><td>328–600</td></tr></table>			P (atm.)	T _s (°C) (min. and max. measured values)	1	250–302	3.5	300–422	8	368–515	13	328–600
P (atm.)	T _s (°C) (min. and max. measured values)												
1	250–302												
3.5	300–422												
8	368–515												
13	328–600												
T of combustion [°C]	Max. measured value = ~ 1,140 ^[1] , 1,140 °C (measured @ 0.1 MPa) ^[7] , 1,925 °C (calcd., @ 0.1 MPa) ^[7] , 2,216 K (adiabatic burning T @ 30 MPa) ^[7]												

Burn rate [mm/s]	Pressure bomb, 1.5 L vol., slit camera, compacted samples in transparent acrylic tubes of 4 or 7 mm diameter @ 150–200 MPa pressure ^[1] :		
	Pressure (MPa)	Burning rate (cm/s)	
		Strands of 4 mm	Strands of 7 mm
	0.1	0.03	0.05
	0.2	0.06	0.1
	0.3	0.07	0.2 @ 0.2 MPa
	0.5	0.1	–
	0.7	0.15	–
	2	0.6	0.7
	3	0.7	–
	4	0.8	1.0
	5	1.0	–
	6	1.5	–
	8	~ 1.8	2
	10	~ 1.9	2.5
<p>Burning rate from Russian FLAME database^[2]: 0.3 mm/s @ 1 atm. pressure^[2], 1.0 mm/s @ 4 atm. pressure^[2], 2.5 mm/s @ 10 atm. pressure^[2], 10.0 mm/s @ 50 atm. pressure^[2], 11.0 mm/s @ 100 atm. pressure^[2]</p> <p>0.3 mm/s @ 0.1 MPa^[7], 0.22 mm/s @ 0.2 MPa^[7], 0.75 @ 0.3 MPa^[7], 0.95 mm/s @ 0.5 MPa^[7], 1.6 mm/s @ 0.75 MPa^[7], 2.2 mm/s @ 1.2 MPa^[7], 4.5 mm/s @ 1.6 MPa^[7], 6 mm/s @ 2 MPa^[7], 7 mm/s @ 3 MPa^[7], 9 mm/s @ 4 MPa^[7], 10 mm/s @ 5 MPa^[7], 15 mm/s @ 6 MPa^[7], 18 mm/s @ 8 MPa^[7], 19 mm/s @ 10 MPa^[7], 30 mm/s @ 15 MPa^[7], 40 mm/s @ 20 MPa^[7], 50 mm/s @ 25 MPa^[7]</p> <p>Combusts readily without smoke^[10]</p>			
Solubility [g/mL]	Recryst. from EtOH ^[1] , soluble in dioxane, DMSO, DMF, H ₂ O, acetone, CHCl ₃ ^[9] , recryst. from ethyl acetate and other common organic solvents ^[5]		

	α-1<i>H</i>-1,2,3,4-Tetrazole^[4]	Tetrazole (α-)^[5]	β-Tetrazole^[6]
Chemical formula	CH ₂ N ₄	CH ₂ N ₄	CH ₂ N ₄
Molecular weight [g mol ⁻¹]	70.07	70.06	70.07
Crystal system	Triclinic	Triclinic	Monoclinic

Space group	<i>P</i> 1		<i>P</i> 2 ₁ or <i>P</i> 2 ₁ / <i>m</i>
<i>a</i> [Å]	3.7250(10)	5.00	4.931(2)
<i>b</i> [Å]	4.7730(10)	5.46	6.451(2)
<i>c</i> [Å]	4.9360(10)	3.75	5.390(1)
α [°]	107.03(2)	130	90
β [°]	107.23(2)	111	116.69(3)
γ [°]	101.57(2)	63	90
<i>V</i> [Å ³]	76.08(4)		
<i>Z</i>	1	1	2
ρ_{calc} [g cm ⁻³]	1.529	1.632	1.52
<i>T</i> [K]	293		
	Crystals grown from <i>n</i> -pentane, colorless prisms		

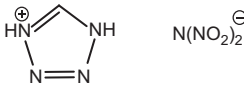
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Tetrazolium dinitramide

Name [German, acronym]: 5 *H*-Tetrazolium dinitramide [tetrazolium dinitramid, HTZ-DN]

Main (potential) use: high explosive, oxidizer

Structural formula:



	Tetrazolium dinitramide		
Formula	CH ₃ N ₇ O ₄		
Molecular mass [g mol ⁻¹]	177.08		
Appearance at RT	colorless crystals ^[1]		
IS [J]	2 (75–125 μm grain size, BAM) ^[1, 2] , 2 ^[3]		
FS [N]	28 (75–125 μm grain size, BAM) ^[1, 2]		
ESD [J]	500 mJ (5–100 μm crystal size, OZM apparatus) ^[1, 2]		
N [%]	36.14		
Ω(CO ₂) [%]	+4.5		
T _{m.p.} [°C]	90 (DSC @ 5 °C/min, pressed Al containers with hole in lid) ^[1] , 70 (DSC @ 5 K/min) ^[2]		
T _{dec.} [°C]	110 (DSC @ 5 °C/min, pressed Al containers with hole in lid) ^[1] , 110 (onset, DSC @ 5 K/min) ^[2] , 130 ^[3]		
ρ [g cm ⁻³]	1.824 (X-ray @ 200 K) ^[1]		
Heat of formation	87.6 kcal/mol (Δ _f H° (s)) ^[1] , 78.6 kcal/mol (Δ _f H° (s), calcd.) ^[2] , 367 kJ/mol (ΔH° _f) ^[2] , –367 kJ/mol (enthalpy of form.) ^[3] , 1,813.3 kJ/kg (Δ _f U° (s), calcd.) ^[2]		
	Calcd. (EXPLO5 5.02)	Lit. values	Exptl.
–Δ _{ex} U° [kJ kg ⁻¹]	6,277 ^[1]		
T _{ex} [K]	4,880 ^[1]		
p _{C-J} [kbar]	365 ^[1]	36.5 GPa (@ 1.82 g cm ⁻³ , calcd., EXPLO) ^[3]	

VoD [m s^{-1}]	9,215 (@ 1.824 g cm^{-3}) ^[1]	9,215 (@ 1.82 g cm^{-3} , calcd., EXPLO) ^[3]	
V_0 [L kg^{-1}]	794 ^[1]		
Solubility [g/mL]	Soluble in EtOH ^[1]		
Hygroscopicity	Hygroscopic ^[1, 2]		

	Tetrazolium dinitramide ^[1]
Chemical formula	$\text{CH}_3\text{N}_7\text{O}_4$
Molecular weight [g mol^{-1}]	177.08
Crystal system	Monoclinic
Space group	$C2/c$ (no. 15)
a [\AA]	6.904(2)
b [\AA]	7.668(2)
c [\AA]	12.200(4)
α [$^\circ$]	90
β [$^\circ$]	93.01(3)
γ [$^\circ$]	90
V [\AA^3]	645.0(3)
Z	4
ρ_{calc} [g cm^{-3}]	1.824
T [K]	200

[1] J. Stierstorfer, *Advanced Energetic Materials Based on 5-Aminotetrazole – Synthesis, Characterization and Scale-Up*, PhD Thesis, LMU München, Munich, **2009**.

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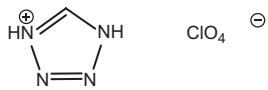
[3] A. Wojewodka, T. Witkowski, *Chemik*, **2013**, 67, 19–24.

1,4*H*-Tetrazolium perchlorate

Name [German, acronym]: Tetrazolium perchlorate, 1*H*-tetrazolium perchlorate
[Tetrazoliumperchlorat, HTz-ClO₄]

Main (potential) use: oxidizer

Structural formula:



	Tetrazolium perchlorate		
Formula	CH ₃ ClN ₄ O ₄		
Molecular ,mass [g mol ⁻¹]	170.52		
Appearance at RT	Colorless plate crystals ^[2]		
IS [J]			
FS [N]			
ESD [J]			
N [%]	32.86		
Ω(CO ₂) [%]			
T _{m,p.} [°C]			
T _{dec.} [°C]			
ρ [g cm ⁻³]	2.021 (X-ray @ 200 K) ^[1, 2]		
Heat of formation			
	Calcd. (EXPL05 6.03)	Lit. values	Exptl.
-Δ _{ex} U° [kJ kg ⁻¹]			
T _{ex} [K]			
p _{C-J} [kbar]			
VoD [m s ⁻¹]			
V ₀ [L kg ⁻¹]			
Hygroscopicity	Hygroscopic ^[1]		

	Tetrazolium perchlorate^[1, 2]
Chemical formula	CH ₃ ClN ₄ O ₄
Molecular weight [g mol ⁻¹]	170.52
Crystal system	Monoclinic
Space group	<i>P</i> 2 ₁ / <i>n</i> (no. 14)
<i>a</i> [Å]	4.9338(4)
<i>b</i> [Å]	7.4893(5)
<i>c</i> [Å]	15.1744(10)
α [°]	90
β [°]	92.073(6)
γ [°]	90
<i>V</i> [Å ³]	560.34(7)
<i>Z</i>	4
ρ_{calc} [g cm ⁻³]	2.021
<i>T</i> [K]	200

[1] J. Stierstorfer, *Advanced Energetic Materials Based on 5-Aminotetrazole – Synthesis, Characterization and Scale-Up*, PhD Thesis, LMU München, Munich, **2009**.

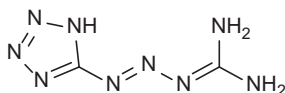
[2] T. M. Klapötke, J. Stierstorfer, *Dalton Trans.*, **2009**, 643–653.

1-[(2E)-3-(1H-Tetrazol-5-yl)triaz-2-en-1-ylidene]methanediamine

Name [German, acronym]: 1-[(2E)-3-(1H-Tetrazol-5-yl)triaz-2-en-1-ylidene]
methanediamine [MTX-1]

Main (potential) use: Possible tetrazene replacement

Structural formula:



	MTX-1	
Formula	C ₂ H ₅ N ₉	
Molecular mass [g mol ⁻¹]	155.13	
Appearance at RT		
IS [J]	0.02 Nm ^[3]	
ESD [J]	3–4 mJ ^[3]	
N [%]	81.27	
Ω(CO ₂) [%]	–67.0	
T _{dec.} [°C]	209 (DSC @ 5 °C/min)	
ρ [g cm ⁻³]	2.47 ^[1] , 2.351 (@ 296 K) ^[2]	
Heat of formation	382 kJ/mol (Δ _f H°) ^[3] , 2,469 kJ/kg (Δ _f H°) ^[3]	
	Calcd. (EXPLO5 6.03)	Exptl.
–Δ _{ex} U° [kJ kg ⁻¹]	2,696	2,254
T _{ex} [K]	2,007	
p _{C-J} [kbar]	338	
VoD [m s ⁻¹]	9,729 (@ 1.9 g cm ⁻³)	
V ₀ [L kg ⁻¹]	847	

[1] Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994–2017 ACD/Labs.

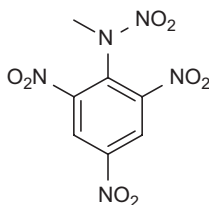
[2] J. W. Fronabarger, M. D. Williams, A. G. Stern, D. A. Parrish, *Centr. Europ. J. Energ. Mat.*, **2016**, 13, 33–52.

[3] R. Meyer, J. Köhler, A. Homburg, *Explosives*, 7th edn., Wiley-VCH, Weinheim, **2016**, pp. 316–317.

Tetryl

- Name [German, acronym]:** 1-Methylnitramino-2,4,6-trinitrobenzene, *N*-methyl-*N*-(2,4,6-trinitrophenyl)nitramide, *N*-methyl-*N*,2,4,6-tetranitrobenzamine, *N*-methyl-*N*,2,4,6-tetranitroaniline, pyronite, tetrylit, tetralite, tetralita, picrylmethylnitramine, 2,4,6-trinitrophenylmethylnitramine, *N*-2,4,6-tetranitro-*N*-methylaniline, 2,4,6-trinitrophenyl-*N*-methylnitramine, tetrylite, tetranitromethylamulene [tetryl, CE]
- Main (potential) use:** Secondary (high) explosive, ingredient in explosive mixtures, component of blasting caps, military boosters, rarely as bursting charge^[9], less commonly in military and commercial detonators^[9], partial substitute for MF charges^[9], was used as booster explosive, in mixtures with TNT and as a base charge in detonators^[21]

Structural formula:



	Tetryl
Formula	C ₇ H ₅ N ₅ O ₈
Molecular mass [g mol ⁻¹]	287.14
Appearance at RT	Light yellow solid ^[14] , light yellow crystalline solid ^[21] , finely divided crystalline powder ^[66] , colorless (freshly prepared, high purity) ^[66] , colorless (highly purified) but rapidly becomes yellow when exposed to light ^[19, 69] , colorless or yellow crystalline solid ^[9] , white crystalline substance, but technical product is bright yellow ^[75]

IS [J]^[10]

3 (<100 μm), 7.85^[1], 5.49^[2], 5.10 (26 cm, 2 kg mass, 20 mg sample, B.M.)^[9, 10, 14], 3.00 (P.A.)^[9, 10], 26 cm (B.M.)^[10, 12], 26 cm (2 kg mass, B.M.)^[33], 25 cm (2.5 kg mass) (P.A.)^[10, 12], 42 cm (tool type 12, ERL)^[12, 13], 28 cm (tool type 12, 5 kg mass, ERL)^[12, 13], 3.99 (8 in, 2 kg mass, 18 mg sample, P.A.)^[10, 14], 13.73 (5 kg, 12 tool)^[15], 9.07 (2.5 kg, 12 tool)^[15], 10.06 (2.5 kg, 12B tool)^[15], 25 cm (5 kg mass)^[18], H_{50} = 42 cm (tool type 12)^[21], H_{50} = 49 cm (tool type 12B)^[21], H_{50} = 28 cm (tool type 12, 5 kg mass)^[23], $H_{50\%}$ = 38 cm (US-NOL apparatus)^[28, 31], $H_{50\%}$ = 32 cm (LASL test)^[24], $H_{50\%}$ = 42 cm (LASL, powdered sample)^[31], $H_{50\%}$ = 94 cm (ERL app. at B.M., powdered sample)^[31], $H_{50\%}$ = 26 cm (B.M. apparatus at P.A., powdered sample)^[31], $H_{10\%}$ = 8 in (P.A., powdered sample)^[31], max. fall for $0/6$ shots = 51 cm (2 kg mass)^[26], 14 cm (10 kg mass)^[26], min. fall for $6/6$ shots ≥ 60 cm (2 kg mass)^[26], >24 cm (10 kg mass)^[26], $H_{50\%}$ = 25 cm (B.M., type 12 tool, 2.5 kg mass, 35 m sample, garnet paper)^[36], H_{50} = 32 cm^[46], 26 cm (NEDED)^[47], 40 cm (NOL)^[47], 37 cm (LANL)^[47], 150 cm ($10/10$ trials positive, 5 kg mass)^[48], 100 cm ($9/10$ trials positive, 5 kg mass)^[48], 50 cm ($5/10$ trials positive)^[48], 40 cm ($3/10$ trials positive, 5 kg mass)^[48], 30–35 cm (2 kg mass, *Stettbacher*)^[49], $H_{50\%}$ = 50 cm (5 kg mass, several decigrams sample contained in small iron cup (0.2 mm thick), covered with 0.2 mm thick iron disc)^[48], $H_{50\%}$ = 38 cm (2.5 kg hammer, 35 mg sample, US Naval lab)^[50], 7.8 Nm^[51], 32 cm (Bruceton method, type 12 tool, 2.5 kg mass, 40 mg sample, 5/0 sandpaper, 25 trials)^[56], Rotter Fol = 123 (yellow, unaged)^[62], Rotter Fol = 100 (orange, unaged)^[62], Rotter Fol = 132 (depth charge, unaged)^[62], Rotter Fol = 111 (recrystallized, unaged)^[62], Rotter Fol = 108 (yellow, aged @ 110 °C for 33 days)^[62], Rotter Fol = 102 (orange, aged @ 110 °C for 33 days)^[62], Rotter Fol = 95 (depth charge, aged @ 110 °C for 33 days)^[62], Rotter Fol = 121 (recrystallized, aged @ 110 °C for 3 days)^[62], H_{50} = 25 cm (2.5 kg mass, type 12 tool)^[63], 27.5 cm (max height for no explosions in 5 trials, 2,000 g mass, BM small impact device)^[67], 40 cm (2 kg mass, explodes)^[75], 8 in (18 mg sample, P.A.)^[76], 26 cm (B.M.)^[76], 32 cm (2.5 kg mass)^[85], A_{d1} = 60%, A_{d2} = 24%, LL = 1.2 m, $A_{50 d1}$ = 2.3 m, $A_{50 d2}$ = 7.3^[86], median height = 112 cm (5 kg mass, 30 mg sample, Rotter apparatus)^[31], \bar{P}_{cr} (critical stress) value for IS = 8.4×10^{-3} kg cm² with a critical thickness h_{cr} of ~ 0.012 mm^[32], drop energy for 50% initiation probability >29.43 J (Julius-Peters apparatus, 25 mg sample)^[33], shock sensitivity dropweight (BAM apparatus) = 6.5–15 Nm^[34]

Rotter impact data: 27 mg sample, Bruceton method/25 drop run to obtain $H_{50\%}$; initiation criteria = 1 mL gas evolved or 0.5 mL accompanied by smoke or evidence of burning in the sample; data from^[90]:

Rotter impact data		US data	
F of I	Gas evolved (mL)	NSWC/NOL, ERL type 12	NWC B.M. type 12
90–110	12–15	38	30, 25

FS [N]	<p>360 (<100 μm), 353^[5], 0.152 @ 0.15 M^[18], $P_{fr,LL} = 400 \text{ MPa}$^[22, 86], $P_{fr,50\%} = 540 \text{ MPa}$^[22, 86], Rotter FS: mean figure of friction (FOF) = 6.3^[35], Rotter FoF = 6.3^[53], 4.5^[53], >360 (BAM, limiting load)^[53], 353 (BAM, limiting load)^[53], BAM mean limiting load >360^[35]</p> <p>Mallet friction sensitivity: steel on steel = 0%^[35], nylon on steel = 0%^[35], wood on soft wood = 0%^[35, 81], wood on hardwood = 0%^[35, 81], wood on Yorkstone = 0%^[35], wood mallet on stone = 50%^[81]</p> <p>Friction pendulum test: crackles with steel shoe^[12, 14, 76], no effect with fiber shoe^[12, 14], does not explode^[69], no detonations with steel shoe^[19]</p>																																									
ESD [J]	<p>0.6 (<100 μm), 5.49^[1], 0.007 (100 mesh, unconfined)^[14], 4.4 (100 mesh, confined)^[14], 0.007 (unconfined)^[76], 0.44 (confined)^[76], 0.025 (8,000 Voltage, 100 sieve, for zero ignition, 500 MMF capacitance, 0.005 in gap setting)^[87]</p> <p>Highest energy (J) for zero ignition probability^[87]:</p> <table><tr><td>Results from^[87]</td><td>Bureau of Mines, 1943</td><td>Bureau of Mines, 1946</td><td>Bureau of Mines, 1954</td><td>NOL, 1959</td></tr><tr><td>0.025</td><td>0.020</td><td>0.007</td><td>0.0005</td><td>1.25</td></tr></table> <p>Spark sensitivity: 0.54 (brass electrode, 3 mm Pb foil thickness)^[21], 2.79 (brass electrode, 10 mm Pb foil thickness)^[21], 0.19 (steel electrode, 1 mm Pb foil thickness)^[21], 3.83 (steel electrode, 10 mm Pb foil thickness)^[21]</p> <p>Highest electrostatic discharge energy @ 5,000 V for zero ignition probability^[29]:</p> <table><tr><td></td><td colspan="2">Highest energy (J) for zero ignition probability</td><td colspan="2">Type of ignition</td></tr><tr><td></td><td>Unconfined</td><td>Confined</td><td>Unconfined</td><td>Confined</td></tr><tr><td>Granular (Tetryl)</td><td>> 11.0</td><td>4.68</td><td>None</td><td>Deton.</td></tr><tr><td>Granular through 100 mesh (Tetryl)</td><td>0.062</td><td>4.38</td><td>Deflag.</td><td>Deton.</td></tr></table> <p>Data from^[88]:</p> <table><tr><td rowspan="2">Material</td><td colspan="3">50% point energy (J)</td></tr><tr><td>3-mil foil</td><td>10-mil foil</td><td>% expl.</td></tr><tr><td>Tetryl (Impact Std)</td><td>9.54</td><td>3.79</td><td>42</td></tr></table>	Results from ^[87]	Bureau of Mines, 1943	Bureau of Mines, 1946	Bureau of Mines, 1954	NOL, 1959	0.025	0.020	0.007	0.0005	1.25		Highest energy (J) for zero ignition probability		Type of ignition			Unconfined	Confined	Unconfined	Confined	Granular (Tetryl)	> 11.0	4.68	None	Deton.	Granular through 100 mesh (Tetryl)	0.062	4.38	Deflag.	Deton.	Material	50% point energy (J)			3-mil foil	10-mil foil	% expl.	Tetryl (Impact Std)	9.54	3.79	42
Results from ^[87]	Bureau of Mines, 1943	Bureau of Mines, 1946	Bureau of Mines, 1954	NOL, 1959																																						
0.025	0.020	0.007	0.0005	1.25																																						
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	Unconfined	Confined	Unconfined	Confined																																						
Granular (Tetryl)	> 11.0	4.68	None	Deton.																																						
Granular through 100 mesh (Tetryl)	0.062	4.38	Deflag.	Deton.																																						
Material	50% point energy (J)																																									
	3-mil foil	10-mil foil	% expl.																																							
Tetryl (Impact Std)	9.54	3.79	42																																							
N [%]	24.39																																									
Ω(CO ₂) [%]	-47.36																																									

$T_{m.p.}$ [°C]	128, 129.5 ^[12, 37, 45, 58, 64, 81, 84] , 130 ^[14, 66] , 130 (pure) ^[32] , 129 (technical grade) ^[32] , 129.45 (pure, partial dec.) ^[19, 75] , 129 (technical grade, partial dec.) ^[19] , 130 ^[33, 76] , 128 (DTA @ 10 °C/min) ^[23] , 130 (dec.) ^[37] , 130 (Thomas Hoover capillary melting point apparatus @ 2 °C/min) ^[58] , 128.07 (endo, onset, DSC @ 10 °C/min, 1–10 mg sample, unsealed but uncovered Al pans) ^[59] , first melts then dec. and explodes on heating ^[66] , 129.5 (with partial dec., monoclinic crystals) ^[69] , 129.5 ^[71] , 129–130 ^[9] , 128.5 (freezing point, chemically pure Tetryl) ^[75] , 127.7 (freezing point, technical Tetryl) ^[75] , 129 ^[85] , 129.45 ^[21]																		
$T_{b.p.}$ [°C]	Dec. ^[45]																		
$T_{dec.}$ [°C]	190 (DSC @ 5 °C/min), 257 (@ 5 °C/s) ^[12] , 238 (@ 10 °C/s) ^[12] , 236 ^[12] , 213 ^[12] , ~ 198 (rapid dec., DTA @ 10 °C/min.) ^[23] , 129 (onset) ^[55] , 195.4 (exo, onset, DSC @ 10 °C/min, 1–10 mg sample, unsealed but uncovered Al pans) ^[59] , 209.2 (exo peak, DTA) ^[61] , 128.8 (DSC, as-received) ^[62] , 128.5 (DSC, Tetryl with low degree of dec.) ^[62] , 128.76 (DSC, Tetryl with medium degree of dec.) ^[62] , 124.4 (DSC, Tetryl with high degree of dec.) ^[62]																		
ρ [g cm ⁻³]	<p>1.731 (@ 295 K)^[5], 1.731 (crystal, @ 295 K)^[20], 1.74 (flotation)^[20, 38], 1.73 (@ TMD)^[12, 19, 20, 32, 33], 1.71 (nominal)^[19, 32], 1.731 (@ TMD)^[12], 1.67 (loaded ρ @ 20 kpsi)^[12], 1.731 (X-ray data @ 21 °C)^[21], 1.74 (flotation @ 21 °C)^[21]</p> <p>ρ @ different loading pressures (pressed):</p> <table border="1"> <thead> <tr> <th>Pressure (kpsi)</th><th>Loading ρ (g cm⁻³)</th></tr> </thead> <tbody> <tr> <td>0</td><td>0.9^[14, 32]</td></tr> <tr> <td>3</td><td>1.40^[14, 19, 21, 31, 32, 76]</td></tr> <tr> <td>5</td><td>1.47^[14, 19, 21, 31, 32, 76]</td></tr> <tr> <td>10</td><td>1.57^[14, 19, 21, 31, 32, 76]</td></tr> <tr> <td>12</td><td>1.60^[14, 19, 31, 32, 76]</td></tr> <tr> <td>15</td><td>1.63^[14, 19, 31, 32, 76]</td></tr> <tr> <td>20</td><td>1.67^[14, 19, 21, 31, 32, 69, 76]</td></tr> <tr> <td>30</td><td>1.71^[14, 21]</td></tr> </tbody> </table> <p>1.73 (crystal)^[14, 31, 69, 76, 85], 1.62 (cast)^[12, 19, 32], 1.731^[46, 81], 1.730^[55, 64], sp. gr. = 1.73^[75], 0.9–1 (gravimetric density)^[75]</p>	Pressure (kpsi)	Loading ρ (g cm ⁻³)	0	0.9 ^[14, 32]	3	1.40 ^[14, 19, 21, 31, 32, 76]	5	1.47 ^[14, 19, 21, 31, 32, 76]	10	1.57 ^[14, 19, 21, 31, 32, 76]	12	1.60 ^[14, 19, 31, 32, 76]	15	1.63 ^[14, 19, 31, 32, 76]	20	1.67 ^[14, 19, 21, 31, 32, 69, 76]	30	1.71 ^[14, 21]
Pressure (kpsi)	Loading ρ (g cm ⁻³)																		
0	0.9 ^[14, 32]																		
3	1.40 ^[14, 19, 21, 31, 32, 76]																		
5	1.47 ^[14, 19, 21, 31, 32, 76]																		
10	1.57 ^[14, 19, 21, 31, 32, 76]																		
12	1.60 ^[14, 19, 31, 32, 76]																		
15	1.63 ^[14, 19, 31, 32, 76]																		
20	1.67 ^[14, 19, 21, 31, 32, 69, 76]																		
30	1.71 ^[14, 21]																		
Heat of formation	4.67 kcal mol ⁻¹ (standard heat of form., ΔH_f°) ^[32] , 7 kcal mol ⁻¹ (standard heat of form., ΔH_f°) ^[32] , 7.6 kcal mol ⁻¹ (ΔH_f°) ^[21] , 4.67–7.6 kcal/mol ^[18, 19] , –69.9 kJ/kg (ΔH_f , ICT thermochemical database) ^[54] , –14 cal/g ^[14, 28] , 27.0 kcal/kg (enthalpy of form.) ^[57] , 9.8 kcal/mol ($\Delta_f H$ (s)) ^[46] , 19.1 kJ/mol (enthalpy of form.) ^[55] , 4.70 kcal/mol (ΔH_B) ^[84] , 7.5 kcal/mol (ΔH_B) ^[84] , 4.67 kcal/mol (ΔH_B) ^[84] , 23.7 kcal/mol (ΔH_B) ^[84] , 5.02 kcal/mol (ΔH_B) ^[84] , –4.67 kcal/mol ($-\Delta H_f$ (heat of form. @ standard conditions)) ^[92]																		

Heat of combustion	2,925 kcal/kg ^[14, 28, 76] , $\Delta H^\circ_c = -836.8$ kcal/mol ^[21] , 2,914 cal/g (@ C ^P) ^[19] , $\Delta Q_c = 840.2$ kcal/mol ^[84] , $\Delta Q_c = 840.22$ kcal/mol ^[84] , $\Delta Q_c = 854.3$ kcal/mol ^[84] , $\Delta Q_c = 837.0$ kcal/mol ^[84] , heat of comb. = 836.78 kcal/mol (@ 1 atm.) ^[91]		
	Exptl. heat of combustion data ^[92] :		
	$-\Delta U_{B/M}$ (cal/g)	$-\Delta U_B$ (kcal/mol)	$-\Delta U_R$ (kcal/mol @ 1 atm. and constant vol.)
			$-\Delta H_R$ (kcal/mol @ 1 atm. and constant pressure)
	2,930.39 ± 1.01	841.46	938.89
			836.78
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl. values
$-\Delta_{\text{ex}} U^\circ$ [kJ kg ⁻¹]	5,619	4,651 ^[3] 1,100 kcal/kg ^[28] 1.44 kcal/g (Q_{max} , calcd.) ^[46] 4,271 J/g (calcd., ICT-code) ^[54] 4,815 ^[55] 976 kcal/kg (@ 0.980 g cm ⁻³ , calcd.) [H ₂ O vapor] ^[57] 1,164 kcal/kg (@ 1.690 g cm ⁻³ , calcd.) [H ₂ O vapor] ^[57] 1,047 cal/g (calcd.) ^[74]	4,773 [H ₂ O (l)] ^[8] 1,080–1,130 cal/g ^[14, 76] 1,450 cal/g [H ₂ O (g)] ^[19] 1,090 cal/g (@ 1.51 g /cc) ^[32] 1,160 cal/g (@ 1.69 g cm ⁻³ , heat of det., sample confined in brass [H ₂ O (g)]) ^[32] 960 cal/g (@ 0.98 g cm ⁻³ , heat of det., sample confined in brass [H ₂ O (g)]) ^[32] 960 kcal/kg (@ 0.980 g cm ⁻³) [H ₂ O vapor] ^[57] 1,160 kcal/kg (@ 1.690 g cm ⁻³) [H ₂ O vapor] ^[57] 1,900 cal/cm ³ (voidless, volumetric heat of explosion) ^[76] 1,720 cal/cm ³ (pressed @ 10,000 psi, volumetric heat of explosion) ^[76]

T_{ex} [K]	4,347	3,370 ^[3] 4,700 (calcd., @ 1.6 g cm ⁻³) ^[28] 3,468 (calcd., ICT code) ^[54] 2,917 (@ 1.70 g cm ⁻³ , $\Delta H_f^0 = 116.1$ kJ/kg, calcd., FORTRAN BKW) ^[72] 3,460 (@ 1.73 g cm ⁻³ , calcd. BKWR) ^[16] 3,480 (@ 1.71 g cm ⁻³ , calcd. BKWR) ^[16] 3,520 (@ 1.68 g cm ⁻³ , calcd. BKWR) ^[16] 3,590 (@ 1.61 g cm ⁻³ , calcd. BKWR) ^[16] 3,750 (@ 1.40 g cm ⁻³ , calcd. BKWR) ^[16] 3,780 (@ 1.36 g cm ⁻³ , calcd. BKWR) ^[16] 3,840 (@ 1.20 g cm ⁻³ , calcd. BKWR) ^[16] 3,840 (@ 1.00 g cm ⁻³ , calcd. BKWR) ^[16] 4,210 (@ 1.73 g cm ⁻³ , calcd. BKWS) ^[16] 4,220 (@ 1.71 g cm ⁻³ , calcd. BKWS) ^[16] 4,240 (@ 1.68 g cm ⁻³ , calcd. BKWS) ^[16] 4,270 (@ 1.61 g cm ⁻³ , calcd. BKWS) ^[16] 4,350 (@ 1.40 g cm ⁻³ , calcd. BKWS) ^[16]	2,017 (@ 1.70 g cm ⁻³) ^[12] 4,837 (@ 1.60 g cm ⁻³) ^[12] 4,837 (@ 1.614 g cm ⁻³ , pressed) ^[28] 4,200 (@ 1.61 g cm ⁻³) ^[16] 4,130 (@ 1.40 g cm ⁻³) ^[16] 4,300 (@ 1.20 g cm ⁻³) ^[16] 4,390 (@ 1.00 g cm ⁻³) ^[16] 4,700 (@ 0.95 g cm ⁻³ , radiation method, det. T) ^[28] 5,100 (@ 1.2 g cm ⁻³ , radiation method, det. T) ^[28] 5,750 (@ 1.55 g cm ⁻³ , radiation method, det. T) ^[28] 4,800 (@ 1.0 g cm ⁻³ , det. T) ^[28] 5,750 (@ 1.5 g cm ⁻³ , det. T) ^[28] 4,800 (@ 0.95 g cm ⁻³) ^[28] 5,750 (@ 1.5 cm ⁻³) ^[28] 3,339 °C (Aranaz) ^[48] 2,911 °C (@ 0.3 g cm ⁻³ , Koehler) ^[48]
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		<p>4,360 (@ 1.36 g cm⁻³, calcd. BKWS)^[16]</p> <p>4,380 (@ 1.20 g cm⁻³, calcd. BKWS)^[16]</p> <p>4,340 (@ 1.00 g cm⁻³, calcd. BKWS)^[16]</p>	
p_{CJ} [kbar]	232	<p>22.11 GPa (@ 1.61 g cm⁻³, calcd., CHEETAH 2.0)^[4]</p> <p>15.41 GPa (@ 1.36 g cm⁻³, calcd., CHEETAH 2.0)^[4]</p> <p>64.6 (@ 0.9 g cm⁻³, calcd., thermochem.)^[40]</p> <p>140 (@ 1.36 g cm⁻³, calcd., thermochem.)^[40]</p> <p>195 (@ 1.51 g cm⁻³, calcd., Ruby code)^[43]</p> <p>193 (@ 1.51 g cm⁻³, calcd., LASL code)^[43]</p> <p>264 (@ 1.731 g cm⁻³, calcd.)^[46]</p> <p>137.0 MPa (calcd., ICT-code)^[54]</p> <p>25.1 GPa (@ 1.70 g cm⁻³, $\Delta H_f^0 = 116.1$ kJ/kg, calcd., FORTRAN BKW)^[72]</p> <p>288 (@ 1.73 g cm⁻³, calcd. BKWR)^[16]</p> <p>270 (@ 1.71 g cm⁻³, calcd. BKWR)^[16]</p> <p>260 (@ 1.68 g cm⁻³, calcd. BKWR)^[16]</p> <p>237 (@ 1.61 g cm⁻³, calcd. BKWR)^[16]</p>	<p>22.64 GPa (@ 1.61 g cm⁻³)^[4, 21]</p> <p>226.4 (@ 1.614 g cm⁻³)^[12]</p> <p>226.4 (@ 1.614 g cm⁻³, pressed)^[28]</p> <p>226 (Tetryl pellets of 5.1 cm diameter (aquarium method), $\rho = 1.614$ g cm⁻³)^[32]</p> <p>~207 (Tetryl pellets of 0.5 in diameter, $\rho = 1.60$ g cm⁻³)^[32]</p> <p>260 (@ 1.71 g cm⁻³)^[12]</p> <p>196 (@ 1.53 g cm⁻³)^[12]</p> <p>239 (@ 1.68 g cm⁻³)^[16]</p> <p>226 (@ 1.61 g cm⁻³)^[16]</p> <p>142 (@ 1.36 g cm⁻³)^[16]</p> <p>58.8 (@ 0.9 g cm⁻³)^[40]</p> <p>151.5 (@ 1.36 g cm⁻³)^[40]</p> <p>0.170 Mbar^[76]</p> <p>276 (voidless)^[76]</p> <p>221 (pressed @ 10,000 psi)^[76]</p>

		<p>178 (@ 1.40 g cm⁻³, calcd. BKWR)^[16]</p> <p>168 (@ 1.36 g cm⁻³, calcd. BKWR)^[16]</p> <p>13 (@ 1.20 g cm⁻³, calcd. BKWR)^[16]</p> <p>97 (@ 1.00 g cm⁻³, calcd. BKWR)^[16]</p> <p>255 (@ 1.73 g cm⁻³, calcd. BKWS)^[16]</p> <p>248 (@ 1.71 g cm⁻³, calcd. BKWS)^[16]</p> <p>239 (@ 1.68 g cm⁻³, calcd. BKWS)^[16]</p> <p>218 (@ 1.61 g cm⁻³, calcd. BKWS)^[16]</p> <p>165 (@ 1.40 g cm⁻³, calcd. BKWS)^[16]</p> <p>157 (@ 1.36 g cm⁻³, calcd. BKWS)^[16]</p> <p>127 (@ 1.20 g cm⁻³, calcd. BKWS)^[16]</p> <p>95 (@ 1.00 g cm⁻³, calcd. BKWS)^[16]</p>	
VoD [m s ⁻¹]	7,038	<p>7,200 (@ 1.65 g cm⁻³)^[3]</p> <p>average value from lit. = 7,680 (@ 1.60–1.71 g cm⁻³)^[27]</p> <p>7,361 (@ 1.61 g cm⁻³, calcd., CHEETAH 2.0)^[4]</p> <p>6,616 (@ 1.36 g cm⁻³, calcd., CHEETAH 2.0)^[4]</p> <p>5,360 (@ 0.9 g cm⁻³, calcd., thermochem.)^[40]</p>	<p>7,581 (@ 1.614 g cm⁻³, pressed)^[25, 28]</p> <p>7,580 (@ 1.71 g cm⁻³)^[12, 16, 25]</p> <p>7,860 (@ 1.70 g cm⁻³)^[25]</p> <p>7,560 (@ 1.70 g cm⁻³)^[25]</p> <p>7,440 (@ 1.6 g cm⁻³)^[25]</p> <p>7,170 (@ 1.53 g cm⁻³)^[12]</p>

		6,680 (@ 1.36 g cm ⁻³ , calcd., thermochem.) ^[40]	7,720 (@ 1.73 g cm ⁻³) ^[6, 16]
		7,780 (@ 1.73 g cm ⁻³ (TMD), calcd., R-P method) ^[42]	7,500 (@ 1.68 g cm ⁻³) ^[6, 16, 25]
		7,770 (@ 1.73 g cm ⁻³ (TMD), calcd., <i>Aizenshtadt</i>) ^[42]	7,400 (@ 1.60 g cm ⁻³) ^[25]
		7,790 (@ 1.73 g cm ⁻³ (TMD), calcd., K-J) ^[42]	7,300 (@ 1.55 g cm ⁻³) ^[25]
		7,020 (@ 1.51 g cm ⁻³ , calcd., Ruby code) ^[43]	7,170 (@ 1.51 g cm ⁻³) ^[25]
		7,000 (@ 1.51 g cm ⁻³ , calcd., LASL code) ^[43]	7,150 (@ 1.506 g cm ⁻³) ^[25]
		7,800 (@ 1.731 g cm ⁻³ , calcd.) ^[46]	6,875 (@ 1.44 g cm ⁻³) ^[25]
		5,510 (@ 1 g cm ⁻³ , calcd., Kamlet method) ^[25]	6,680 (@ 1.36 g cm ⁻³) ^[6, 16, 25]
		7,370 (@ 1.6 g cm ⁻³ , calcd., Kamlet method) ^[25]	6,291 (@ 1.22 g cm ⁻³) ^[25]
		5,150 (@ 1 g cm ⁻³ , calcd., Urizar method) ^[25]	5,360 (@ 0.90–0.95 g cm ⁻³) ^[25]
		7,350 (@ 1.6 g cm ⁻³ , calcd., Urizar method) ^[25]	5,390 (@ 0.95 g cm ⁻³) ^[25]
		7,550 (@ 1.50 g cm ⁻³ , calcd. K-W eqn.) ^[68]	6,340 (@ 1.2 g cm ⁻³) ^[6, 16]
		7,629 (@ 1.70 g cm ⁻³ , $\Delta H_f^0 = 116.1$ kJ/kg, calcd., FORTRAN BKW) ^[72]	7,580 (@ 1.61 g cm ⁻³) ^[16]
		7,750 (@ 1.73 g cm ⁻³ , calcd. BKWR) ^[16]	7,910 (@ 1.73 g cm ⁻³) ^[7]
		7,690 (@ 1.71 g cm ⁻³ , calcd. BKWR) ^[16]	7,350 (@ 1.71 g cm ⁻³) ^[9]
		7,600 (@ 1.68 g cm ⁻³ , calcd. BKWR) ^[16]	7,570 (@ 1.62 g cm ⁻³) ^[11, 39]
			7,850 (@ 1.71 g cm ⁻³ , 1.0 in charge diameter, pressed, no confinement) ^[14]
			7,626 (based on sand expt.) ^[27]
			7,850 (@ 1.71 g cm ⁻³ , pressed @ 30,000 psi) ^[69]
			7,350 (@ 1.71 g cm ⁻³) ^[9]
			7,160 (@ 1.50 g cm ⁻³) ^[81]
			7,229 (cast Tetryl) ^[48]

		<p>7,390 (@ 1.61 g cm⁻³, calcd. BKWR)^[16]</p> <p>6,780 (@ 1.40 g cm⁻³, calcd. BKWR)^[16]</p> <p>6,670 (@ 1.36 g cm⁻³, calcd. BKWR)^[16]</p> <p>6,240 (@ 1.20 g cm⁻³, calcd. BKWR)^[16]</p> <p>5,750 (@ 1.00 g cm⁻³, calcd. BKWR)^[16]</p> <p>7,810 (@ 1.73 g cm⁻³, calcd. BKWS)^[16]</p> <p>7,740 (@ 1.71 g cm⁻³, calcd. BKWS)^[16]</p> <p>7,630 (@ 1.68 g cm⁻³, calcd. BKWS)^[16]</p> <p>7,380 (@ 1.61 g cm⁻³, calcd. BKWS)^[16]</p> <p>6,700 (@ 1.40 g cm⁻³, calcd. BKWS)^[16]</p> <p>6,590 (@ 1.36 g cm⁻³, calcd. BKWS)^[16]</p> <p>6,150 (@ 1.20 g cm⁻³, calcd. BKWS)^[16]</p> <p>5,680 (@ 1.00 g cm⁻³, calcd. BKWS)^[16]</p>	<p>5,400 (@ 0.90 g cm⁻³, half-meter lengths, contained in extra-light Pb tubing, 12 ounces to the foot)^[49]</p> <p>7,530 (@ 1.682 g cm⁻³, Dautriche method, Cu tubes, 10 mm diameter, compressed under 2,500 kg/cm²)^[49]</p> <p>7,440 (@ 1.682 g cm⁻³, Dautriche method, Cu tubes, 10 mm diameter, compressed under 2,500 kg/cm²)^[49]</p> <p>5,176 (@ 0.9 g cm⁻³)^[40]</p> <p>6,751 (@ 1.36 g cm⁻³)^[40]</p> <p>7,850 (@ 1.710 g cm⁻³)^[41]</p> <p>5,680 (@ 1 g cm⁻³)^[25]</p> <p>7,440 (@ 1.6 g cm⁻³)^[25]</p> <p>7,300 (@ 1.50 g cm⁻³)^[68]</p> <p>7,573 (@ 1.71 g cm⁻³)^[34]</p> <p>7,150 (@ 1.52 g cm⁻³, after 16 h @ -54 °C)^[14]</p> <p>7,170 (@ 1.53 g cm⁻³, after 16 h @ 21 °C)^[14]</p> <p>7,560 (@ 1.70 g cm⁻³)^[72]</p> <p>7,500 (@ 1.63 g cm⁻³)^[75]</p>
V_0 [L kg ⁻¹]	626	710 (@ 0 °C) ^[3]	<p>760^[12, 14, 19, 76]</p> <p>861^[17]</p> <p>620 (@ 1.55 g cm⁻³, using Dolgov's bomb) [H₂O (l)]^[29, 30]</p> <p>740 (@ 1.55 g cm⁻³, using Dolgov's bomb) [H₂O (g)]^[29, 30]</p> <p>765^[75]</p>

Low velocity detonation in Tetryl^[19]:

Particle size in mm	Minimum diameter for low velocity detonation	Minimum diameter from normal detonation in mm	Transition diameter in mm	Minimum low velocity detonation in km/s	Maximum low velocity detonation in km/s
0.5	7	13	13	1.4	2.1
0.8	9	15	16	1.3	2.3
1.3	12	20	21	1.3	2.2

Values calculated using hydrodynamic theory of detonation equations^[28]:

ρ of charge (g cm^{-3})	Detonation pressure (kg/cm^2)	VoD (m/s)	Detonation temperature (K)
1.00	91,800	5,480	4,400
1.28	160,400	6,510	4,740
1.45	218,100	7,220	4,980
1.54	242,500	7,375	5,100
1.61	259,100	7,470	5,140

Loading $\rho = 1.50 \text{ g cm}^{-3}$, det. $T = 4,480 \text{ }^\circ\text{C}$, VoD = 7,125 m/s, pressure (10 atm.) = 1.48^[28]

Experimental temperatures of detonation by the radiation method in air at atmospheric pressure^[28]:

Average particle diameter (microns)	ρ (g cm^{-3})	Average temp. of det. (K)
10	0.70	4,120
10	1.60	6,050
800 (20 mesh)	0.95	4,460
800 (20 mesh)	1.62	6,200

Experimental temperatures of detonation using the luminosity method, unsheathed explosions in air^[28]:

Loading ρ (g cm ⁻³)	Radiation slit width (mm)	Average temp. of det. (K)
1.30	1.0	6,000
1.60	1.0	4,900

Experimental VoD (sweep-trace of cathode ray tube by electrical signals; separation of original stations = 10 cm, station 1 located 5 cm from detonator, charge diameter = 1.92 cm)^[28]:

Average particle diameter (microns)	ρ (g cm ⁻³)	VoD (m/s)
10	0.70	4,310
10	1.60	7,200
800 (20 mesh)	0.95	4,940
800 (20 mesh)	1.62	7,470

VoD of Tetryl of size 10 microns propagated at a distance of ~ 10 cm^[28]:

ρ (g cm ⁻³)	0.85	1.04	1.26	1.57
VoD (m/s)	5,040	5,750	6,415	7,405

VoDs for pelleted Tetryl in air and propane as well as cemented vs. noncemented charges. Station distance of 8.8 cm for $\rho = 1.62$ g cm⁻³ charges and 7.1 cm for $\rho = 1.22$ g cm⁻³ charges^[28]:

ρ (g cm ⁻³)	Pellet boundary	Surround and impregnant	VoD (m/s)
1.62	Cemented	Air	7,341
1.62	Noncemented	Air	7,364
1.62	Cemented	Propane	7,449
1.22	Noncemented	Air	6,502
1.22	Noncemented	Propane	6,525

VoD after storing Tetryl; Tetryl pellets, charges = sticks of $1\frac{1}{8}$ in in diameter and 18 in long, drum camera apparatus^[28]:

Storage	ρ (g cm ⁻³)	Detonation rate (m/s)
16 h @ -65°F	1.52	7,150
16 h @ +70 °F	1.53	7,170

VoD using different confining vessels^[28]:

Confining vessel	Charge diameter (mm)	Wall thickness (mm)	Charge ρ (g cm ⁻³)	VoD (m/s)
Paper wall	5	0.08	0.240	2,605
Glass wall	5	1.0	0.240	2,900
Copper wall	7	0.23	1.69	7,622
Copper wall	21	2	1.69	7,625

Radiation T observed without slit aperture, for interval after detonation of 18 ms: loading $\rho = 1.64$ g cm⁻³, average $T = 5,335$ K^[28]

C-J particle velocity (U_{C-J}):

1.83 mm/ μ s (@ 1.51 g cm⁻³, calcd., Ruby code)^[43]

1.827 mm/ μ s (@ 1.51 g cm⁻³, calcd., LASL code)^[43]

VoD values (m/s) in cylindrical charges of 3.17 cm diameter, unconfined, pressed Tetryl, $\rho = 1.506$ g cm⁻³, no. shots fired = 10^[70]: 7,175; 7,170; 7,162; 7,155; 7,153; 7,151; 7,150; 7,148; 7,142; 7,135, mean value = 7,250 m/s^[70]

Critical T [°C]	187 (T_m) ^[21]	
Critical diameter [cm]	Critical detonation diameter d_{c0} [mm] and specific surface area, S_g [cm ² g ⁻¹] ^[55] :	
	S_g (cm ² g ⁻¹)	d_{c0} (mm)
	Monodisperse Tetryl (fractions)	
	200 (400–500 μ m)	5.79
	390 (200–315 μ m)	3.95
	840 (90–160 μ m)	3.04

	<p>d_{c0} (mm) @ mean crystal size (μm)^[55]: 0.80 @ 3, 1.30 @ 10, 1.75 @ 20^[55]</p> <p>Data from^[80]:</p> <table><tr><th>Particle size (μ)</th><th>ρ_0 (g/cm³)</th><th>Approx. d_c (mm)</th></tr><tr><td>50–150</td><td>1.65</td><td>0.55–0.58</td></tr><tr><td>50–150</td><td>1.58</td><td>0.70</td></tr><tr><td>1–10</td><td>1.16</td><td>0.94</td></tr></table> <p>Failure diameters of lead and booster explosives^[76]:</p> <table><tr><th rowspan="2">Bare, in</th><th colspan="5">Confinement, in</th></tr><tr><th>Fabric (detonating cord)</th><th>Lucite</th><th>Aluminum (0.006 walls)</th><th>Lead (MDF)</th><th>Heavy brass or steel</th></tr><tr><td><0.50</td><td>–</td><td>–</td><td>0.10–0.13</td><td>–</td><td><0.08</td></tr></table>	Particle size (μ)	ρ_0 (g/cm ³)	Approx. d_c (mm)	50–150	1.65	0.55–0.58	50–150	1.58	0.70	1–10	1.16	0.94	Bare, in	Confinement, in					Fabric (detonating cord)	Lucite	Aluminum (0.006 walls)	Lead (MDF)	Heavy brass or steel	<0.50	–	–	0.10–0.13	–	<0.08
Particle size (μ)	ρ_0 (g/cm ³)	Approx. d_c (mm)																												
50–150	1.65	0.55–0.58																												
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1–10	1.16	0.94																												
Bare, in	Confinement, in																													
	Fabric (detonating cord)	Lucite	Aluminum (0.006 walls)	Lead (MDF)	Heavy brass or steel																									
<0.50	–	–	0.10–0.13	–	<0.08																									
Trauzl test [cm ³ , % TNT]	125–142% TNT ^[19] , 340–350 cc ^[31] , 125% TNT ^[9, 14, 32] , 125–145% TNT ^[27] , 13.8 cc (small Trauzl test) ^[49, 67] , 360 cm ³ (10 g sample, sand tamping) ^[49] , 375 cc (10 g sample) ^[48] , 70% PETN ^[49] , 340 cc ^[75] , 410 ^[82]																													
Sand test [g]	54.2 g (200 g bomb) ^[9, 14] , 113–123% TNT ^[19, 27] , 126% TNT ^[33] , 47.7 g sand crushed (1,700 g bomb, 0.4 g Tetryl) ^[27] , 65.9 g (amount of sand crushed finer than 30 mesh, by total charge consisting of base charge of 0.50 g Tetryl and 0.30 g priming charge of MF) ^[67] , 54.2 g (amount of sand crushed finer than 30 mesh, by base charge of 0.50 g Tetryl) ^[67] , rel. strength cf. TNT = 1.24 ^[67]																													
Lead block compression test	Small lead block compression test (50 g Tetryl exploded by detonator on top of lead cylinder 64 mm long): 16.6 mm shortening ^[49]																													
Ballistic mortar test	126–132% TNT ^[19, 27] , 130% TNT ^[9, 14, 32, 33]																													
Initiation efficiency	Minimum charge for detonation of Tetryl requires ^[48] : 0.20–0.29 g MF ^[19] , 0.29 g MF ^[48] , 0.02 g silver fulminate ^[48] , 0.008 g cadmium fulminate ^[48] , 0.045 g mercurous azide ^[48] , 0.02 g silver azide ^[48] , 0.025–0.10 g LA ^[19] , 0.025 g LA ^[48, 49] , 0.1 g cadmium azide ^[48] , 0.01 g cadmium azide ^[49] , 0.07 g thallium azide ^[49] , 0.025 g cuprous azide ^[49] , 0.025 g copper fulminate ^[49] , 0.30 g thallium fulminate ^[49] , readily initiated by 0.10 g LA or 0.20 g MF in sand test ^[69] , Tetryl containing 60% water cannot be detonated by a commercial detonator ^[19] , 0.1 g minimum detonating charge of LA ^[76]																													

	<p>Minimum charges of fulminate-chlorate (90:10) initiator necessary to cause complete detonation of Tetryl or TNT/Tetryl mixtures^[48]:</p> <table><tr><th>TNT-Tetryl mixture</th><th>Weight of initiator required (g)</th><th>TNT-Tetryl mixture</th><th>Weight of initiator required (g)</th></tr><tr><td>90–10</td><td>0.22</td><td>50–50</td><td>0.20</td></tr><tr><td>80–20</td><td>0.21</td><td>0–100</td><td>0.19</td></tr></table> <p>Minimum initiating charge (g) required to detonate Tetryl (0.4 g Tetryl loaded into detonator capsule, pressed down, initiator added on top, covered with short reinforcing cap, pressed with 200 atm./in²)^[49]: 0.04 g cyanuric azide^[49], 0.24 g MF^[49]</p> <p>Minimum initiating charge required to detonate Tetryl (0.5 g Tetryl in No. 8 detonator shell, primary explosive added on top, both compressed under reinforcing capsule @ 3,400 lb/in²)^[49]: 0.075 g DDNP^[49], 0.165 g MF^[49], 0.03 g LA^[49]</p> <p>Minimum detonating charge required to detonate Tetryl (0.4 g, with primary explosive, compressed in detonator capsule under 1,000 lb/in²)^[49]: 0.24 g fulminate (with reenforcing cap)^[49], 0.05 g HMTD (with reinforcing cap)^[49], 0.06 g HMTD (without reinforcing cap)^[49]</p> <p>1 g Tetryl compressed in No. 8 detonator shell under 500 kg/cm² pressure with TATNB compressed on top of it under 300 kg/cm² required 0.01 g TATNB for complete detonation^[49]</p> <p>Minimum weight of priming charge which causes complete detonation of the base charge^[67]: 0.075 g DDNP^[67], 0.165 g MF^[67], 0.03 g LA^[67] Max. initiating charge of MF for pressed Tetryl = 0.29 g^[75] and 0.03 g for LA^[75]</p>	TNT-Tetryl mixture	Weight of initiator required (g)	TNT-Tetryl mixture	Weight of initiator required (g)	90–10	0.22	50–50	0.20	80–20	0.21	0–100	0.19	
TNT-Tetryl mixture	Weight of initiator required (g)	TNT-Tetryl mixture	Weight of initiator required (g)											
90–10	0.22	50–50	0.20											
80–20	0.21	0–100	0.19											
Gap test	9.5 kbar, loading charge = 1.62 g cm ⁻³ ^[34] air gap (inches) ^[85] : 0.096 @ -60 °C ^[85] , 0.127 @ ambient T ^[85] , 0.156 @ 100 °C ^[85]													
US NOL gap test	6.63 cm gap value (@ 1.615 g cm ⁻³ , pressed Tetryl) ^[28, 50]													
LSGT [cm]	<p>G₅₀ = 69.21 mm, L₉₅ = 0.61 mm (@ 0.85 g cm⁻³)^[21], G₅₀ = 60.60 mm, L₉₅ = 0.63 mm (@ 1.666 g cm⁻³)^[21], G₅₀ = 59.38 mm, L₉₅ = 0.18 mm (@ 1.682 g cm⁻³)^[21], 52 mm (NOL)^[47], 54 mm (LANL)^[47], L_g = 234 in × 10² (@ 1.682 g cm⁻³, 97.2% TMD, LASL LSGT, pressed Tetryl)^[58], L_g = 221 × 10² in (extrapolated, NSWC LSGT)^[58], ρ₀ = 1.43 g/cc, 82.4% TMD, 50% pressure (P_g) = 9.0 kbar^[80]</p> <p>Data from^[19]:</p> <table><tr><td rowspan="4">LANL LSGT</td><td>Density (g/cm³)</td><td>% voids</td><td>Sensitivity (mm)</td></tr><tr><td>1.690 (not pressed)</td><td>2.3</td><td>59.82</td></tr><tr><td>1.666 (pressed)</td><td>3.7</td><td>60.60</td></tr><tr><td>0.85 (bulk)</td><td>50.9</td><td>69.2</td></tr></table>	LANL LSGT	Density (g/cm ³)	% voids	Sensitivity (mm)	1.690 (not pressed)	2.3	59.82	1.666 (pressed)	3.7	60.60	0.85 (bulk)	50.9	69.2
LANL LSGT	Density (g/cm ³)		% voids	Sensitivity (mm)										
	1.690 (not pressed)		2.3	59.82										
	1.666 (pressed)		3.7	60.60										
	0.85 (bulk)	50.9	69.2											

	Regular test, I = isostatic press, H = hydraulic press, data from ^[80] :						
	Density		50% point		Particle size (microns)		
	g/cc	% TMD	Cards	kbar			
	1.43I	82.6	294	9	460 (charges contain 0.5% graphite)		
	1.49I	86.0	283	10	460		
	1.62 H	93.4	261	(12)	X-8		
	1.64I	94.9		14	460		
SSGT [cm]	$G_{50} = 7.44$ mm, $L_{95} = 0.05$ mm (@ 0.93 g cm ⁻³) ^[21] , $G_{50} = 4.04$ mm, $L_{95} = 0.20$ mm (@ 1.678 g cm ⁻³) ^[21] , $G_{50} = 3.83$ mm, $L_{95} = 0.30$ mm (@ 1.684 g cm ⁻³) ^[21] , 7.4 mm (NOL) ^[47] , 3.7 mm (LANL) ^[47] , $P_{90} = 10.64$ kbar (P_{90} = pressure to 90% of TMD, NSWC small-scale gap test) ^[56] Data from ^[19] :						
		Density (g/cc)	% Voids	Sensitivity (mm)			
NSWC SSGT	1.687	2.5	7.80				
	1.434	17.1	11.96				
LANL SSGT	1.684 (pressed)	2.7	3.84				
	1.676 (pressed)	3.1	4.04				
	0.93 (bulk)	46.2	7.44				
	Tetryl, yellow, TMD = 1.73 g cm ⁻³ , data from ^[79] :						
Loading pressure (kpsi)	Density (g/cm ³)		% TMD	Sensitivity (DBg)			
	AVG.	S		AVG.	g	S_m	N
4	1.434	–	82.9	3.267	0.0475	0.0243	20
8	1.535	–	88.7	3.468	0.0477	0.0297	20
10	1.527	0.0096	88.3	3.586	0.1307	0.0434	46
16	1.623	–	93.8	4.360	0.1631	0.0901	20
32	1.687	–	97.5	5.133	0.0242	0.0205	20
64	1.732	–	100.1	6.093	0.0242	0.0202	20

Tetryl (graphited), TMD = 1.73 g/cm³ (the TMD of pure Tetryl is used since graphited Tetryl can contain either calcium stearate ($\rho = 1.040$) or graphite ($\rho = 2.25$), or both in any combination, up to a total of 2% by weight)^[79]:

Loading pressure (kpsi)	Density (g/cm ³)		% TMD	Sensitivity (DBg)			
	AVG.	s		AVG.	<i>g</i>	<i>s_m</i>	<i>N</i>
3	1.423	0.0073	82.3	3.291	0.0369	0.0220	28
5.3	1.503	0.0032	86.9	3.684	0.0282	0.0209	28
8	1.549	—	89.5	4.239	0.0098	0.0337	28
24	1.660	0.0015	96.0	5.081	0.0392		28

Tetryl (graphited), TMD = 1.73 g/cm³ (the TMD of pure Tetryl is used since graphited Tetryl can contain either calcium stearate ($\rho = 1.040$) or graphite ($\rho = 2.25$), or both in any combination, up to a total of 2% by weight)^[79]:

Loading pressure (kpsi)	Density (g/cm ³)		% TMD	Sensitivity (DBg)			
	AVG.	s		AVG.	<i>g</i>	<i>s_m</i>	<i>N</i>
4	1.445	0.0042	83.5	3.450	0.0352	0.0220	23
8	1.541	0.0057	89.1	4.103	0.0123	0.0132	23
16	1.630	0.0038	94.2	4.659	0.0400	0.0237	23
32	1.696	0.0022	98.0	5.465	0.0489	0.0297	23
64	1.737	0.0022	100.4	6.503	0.0748	0.0404	23

Tetryl (graphited), TMD = 1.738, (1) = no mixed response zone^[79]:

Loading pressure (kpsi)	Density (g/cm ³)		% TMD	Sensitivity (DBg)			
	AVG.	s		AVG.	<i>g</i>	<i>s_m</i>	<i>N</i>
8	1.545	0.0030	88.9	4.112	0.0037	0.0047	20
16	1.623	0.0023	93.4	4.487	—	—	20 (1)
32	1.695	0.0021	97.5	5.243	—	—	20 (1)

$\rho_0 = 1.43$ g/cc, 82.4% TMD, 50% pressure (P_g) = 9.9 kbar (interpolated)^[80]

4.36 DBg @ 1.623 g cm⁻³ (110 MPa)^[83]

5 s explosion T [°C] Explosion T [°C]	<p>257 (dropping on hot Cu surface)^[32]</p> <p>340 (0.1 s, no cap used)^[14], 314 (1 s)^[14, 76], 238 (10 s)^[14], 236 (15 s)^[14], 234 (20 s)^[14], 40 s @ 180 °C^[19], 340 (0.1 s)^[76], 242 (Wood's metal bath, 40 mg)^[83] explosion T (°C)/time of exposure (s) (25 mg sample, ignition or deflagration occurred): 346/0.325, 314/0.742, 285/1.45, 269/2.22, 264/no action^[30], 210 (DTA/TG @ 6 °C/min)^[34], 190–194 (0.5 g sample, heating rate 20 °C/min)^[19, 32], 196 (bath heating rate @ 20 °C/min)^[26], 187 (bath heating rate @ 5 °C/min)^[26], 302 (0.4 s, dropping on hot Cu surface)^[19, 32], 280 (1.1 s, dropping on hot Cu surface)^[19, 32], 260 (2.0 s, dropping on hot Cu surface)^[19, 32], 236 (6.2 s, dropping on hot Cu surface)^[19, 32]</p> <p>Heat initiation of confined Tetryl; explosion times for confined samples (25 mg Tetryl in Cu shells, 0.635 mm diameter submerged in hot Wood's metal bath)^[19]:</p> <table><tr><th>T (°C)</th><th>Time to explosion (s)</th></tr><tr><td>360</td><td>0.325</td></tr><tr><td>346</td><td>0.425</td></tr><tr><td>329</td><td>0.582</td></tr><tr><td>285</td><td>1.45</td></tr><tr><td>269</td><td>2.22</td></tr><tr><td>264</td><td>Does not detonate</td></tr></table>	T (°C)	Time to explosion (s)	360	0.325	346	0.425	329	0.582	285	1.45	269	2.22	264	Does not detonate						
T (°C)	Time to explosion (s)																				
360	0.325																				
346	0.425																				
329	0.582																				
285	1.45																				
269	2.22																				
264	Does not detonate																				
5 s ignition T [°C] Ignition T [°C]	<p>257 (ignites, USA value)^[14, 28, 60, 76], 190–257 (ignites, Russian value)^[28], 267^[76]</p> <p>180 (in 40 s)^[32], 196 (heated form 100 °C @ 20 °C/min)^[48], 187 (heated form 100 °C @ 5 °C/min)^[48], 180^[50], 175 (calorimetric measurement)^[60], 190–194^[cited in 60], 257 (5 s)^[9], 238 (10 s)^[76]</p>																				
Detonation T [°C]	<p>T (°) and explosion time (s), 25 mg sample^[65]:</p> <table><tr><th>T (°C)</th><th>Time (s)</th><th>T (°C)</th><th>Time (s)</th></tr><tr><td>360</td><td>0.325</td><td>285</td><td>1.45</td></tr><tr><td>346</td><td>0.425</td><td>269</td><td>2.22</td></tr><tr><td>329</td><td>0.582</td><td>264</td><td>No explosion</td></tr><tr><td>314</td><td>1.45</td><td></td><td></td></tr></table> <p>~234^[66]</p>	T (°C)	Time (s)	T (°C)	Time (s)	360	0.325	285	1.45	346	0.425	269	2.22	329	0.582	264	No explosion	314	1.45		
T (°C)	Time (s)	T (°C)	Time (s)																		
360	0.325	285	1.45																		
346	0.425	269	2.22																		
329	0.582	264	No explosion																		
314	1.45																				
100 °C heat test [% mass loss]	0.1% loss in first 48 h ^[14] , 0.0% loss in second 48 h ^[14] , no explosion in 100 h ^[14]																				
75 °C Int. heat test	0.01% loss in 48 h ^[14]																				

Abel heat test time (min)	<30 (recryst. Tetryl) ^[44] , <30 (recryst. Tetryl with 0.1% 2,4,6-trinitroresorcinol) ^[44] , 16.5 (recryst. Tetryl with 1% 2,4,6-trinitroresorcinol) ^[44] , 11 (recryst. Tetryl with 1% 2,4,6-trinitroanisole) ^[44] , 7 (recryst. Tetryl with 1% 2,4,6-trinitroresorcinol and 1% 2,4,6-trinitroanisole) ^[44] , 18 (recryst. Tetryl with 0.1% Shellac) ^[44] , 11.5 (recryst. Tetryl with 1% Shellac) ^[44] , Tetryl withstood Abel test @ 100 °C for 20 min after heated for 2 years @ 60 °C ^[75]																		
LLNL reactivity test	0.036 cm ³ gas evolved per 0.25 g sample in 12 h @ 120 °C ^[23]																		
Thermal stability	<p>Prolonged heating @ 120 °C forms PA^[19], ammunition that contains Tetryl cannot be stored >125 °C^[19]</p> <p>7 (°C) of sample @ ignition/time of heating bath after it reached 100 °C (min)^[31], 232/5.87 (explosion), 214/5.27 (explosion)^[31]</p> <p>0.36% mass loss @ 120 °C, 48 h (TG)^[61], no serious dec. if stored at RT^[66]</p> <p>Withstands storage without significant decrease in stability at: 100 °C for 100 h^[69], 75 °C for 6 months^[69], 65 °C for 12 months^[69], magazine temperature for 20 years^[69], completely stable @ T<120 °C^[9], sufficient stability for long-term storage under normal conditions^[75], 0.3% mass loss on heating @ 75 °C for 320 days^[75], 11.5% mass loss on heating @ 110 °C for 16 days^[75]</p>																		
Vacuum stability test	<p>0.3 cc/40 h @ 100 °C^[14], 1.0 cc/40 h @ 120 °C^[14, 76], 11+ cc/40 h @ 150 °C^[14], 0.14 cc gas/48 h/g @ 100 °C^[85], >30 cc gas/h/g @ 260 °C^[85]</p> <p>Less stable than TNT^[19], 0.4–1.0 mL/g of gas evolved after 48 h @ 120 °C^[21], 1.10 mL/5 g @ 120 °C, 48 h^[61], 0.16 cm³ gas produced @ 100 °C (recryst. Tetryl)^[44], 0.15 cm³ gas produced @ 100 °C (recryst. Tetryl)^[44], 11.08 cm³ gas produced @ 100 °C (recryst. Tetryl and Shellac 50%, sample melted during test and bubbles observed)^[44]</p> <p>VST data for yellow and orange Tetryl aged @ 115 °C, for 40 h, 5 g sample (aged samples were 3 g), normalized gas volume cm³/g^[62]:</p> <table border="1"> <tr> <th>Tetryl sample</th><th>As received (0 days @ 115 °C)</th><th>Low-aging (4 days @ 115 °C)</th><th>Medium aging (11 days @ 115 °C)</th><th>High aging (4 days @ 115 °C)</th></tr> <tr> <td>Yellow Tetryl</td><td>0.29</td><td>0.36</td><td>0.97</td><td>3.48</td></tr> <tr> <td>Orange Tetryl</td><td>0.39</td><td>0.49</td><td>1.20</td><td>4.11</td></tr> </table>				Tetryl sample	As received (0 days @ 115 °C)	Low-aging (4 days @ 115 °C)	Medium aging (11 days @ 115 °C)	High aging (4 days @ 115 °C)	Yellow Tetryl	0.29	0.36	0.97	3.48	Orange Tetryl	0.39	0.49	1.20	4.11
Tetryl sample	As received (0 days @ 115 °C)	Low-aging (4 days @ 115 °C)	Medium aging (11 days @ 115 °C)	High aging (4 days @ 115 °C)															
Yellow Tetryl	0.29	0.36	0.97	3.48															
Orange Tetryl	0.39	0.49	1.20	4.11															
Vapor pressure [atm. @ °C]	5.7 × 10 ⁻⁹ Torr @ 25 °C ^[45] , 5.69 × 10 ⁻⁹ Torr @ 25 °C ^[64] , 5.69 × 10 ⁻⁹ mm Hg @ 25 °C ^[71]																		
Volatility	0.00 @ 25 °C ^[14]																		

Burn rate [mm/s]	Flammable and burns readily ^[66]																											
	Mass burning rate of volatile explosives, data from ^[78] :																											
	<table><tr><th colspan="7">m, gm cm⁻² s⁻¹</th></tr><tr><td>1 atm.</td><td>10 atm.</td><td>40 atm.</td><td>100 atm.</td><td>200 atm.</td><td>400 atm.</td><td>1,000 atm.</td></tr><tr><td>0.067</td><td>0.312</td><td>0.815</td><td>1.55</td><td>2.49</td><td>4.60</td><td>11.4</td></tr></table>							m , gm cm ⁻² s ⁻¹							1 atm.	10 atm.	40 atm.	100 atm.	200 atm.	400 atm.	1,000 atm.	0.067	0.312	0.815	1.55	2.49	4.60	11.4
	m , gm cm ⁻² s ⁻¹																											
	1 atm.	10 atm.	40 atm.	100 atm.	200 atm.	400 atm.	1,000 atm.																					
0.067	0.312	0.815	1.55	2.49	4.60	11.4																						
Burn rate and equilibrium combustion temperature ^[78] : $T_e = 2,775$ K ^[78] , $m = 1.55$ g cm ⁻² s ⁻¹ (100 atm.) ^[78]																												
Dependence of mass burning rate of volatile explosives on the relative density of the charge ^[78] :																												
	<table><tr><td></td><th colspan="6">$m(\delta)$</th></tr><tr><td>p, atm.</td><td>δ</td><td>0.49</td><td>0.54</td><td>0.56</td><td>0.62</td><td>0.64</td></tr><tr><td>1</td><td>m, gm cm⁻² s⁻¹</td><td>0.060 0.065</td><td>0.065</td><td>0.062</td><td>0.066</td><td>0.064</td></tr></table>							$m(\delta)$						p , atm.	δ	0.49	0.54	0.56	0.62	0.64	1	m , gm cm ⁻² s ⁻¹	0.060 0.065	0.065	0.062	0.066	0.064	
	$m(\delta)$																											
p , atm.	δ	0.49	0.54	0.56	0.62	0.64																						
1	m , gm cm ⁻² s ⁻¹	0.060 0.065	0.065	0.062	0.066	0.064																						

Solubility [g/mL]	Solubility of Tetryl (g) in 100 g (%) solvent, data from ^[14] :							
	Water		Carbon tetrachloride		Ether		95% Alcohol	
	°C	%	°C	%	°C	%	°C	%
	0	0.0050	0	0.007	0	0.188	0	0.320
	20	0.0075	20	0.015	10	0.330	10	0.425
	40	0.0110	40	0.058	20	0.418	20	0.563
	80	0.0810	60	0.154	30	0.493	30	0.76
	100	0.184					50	1.72
							75	5.33
	Chloroform		Carbon disulfide		Ethylene dichloride		Acetone	
	°C	%	°C	%	°C	%	°C	%
	0	0.28	0	0.009	25	4.5	20	75
	20	0.39	10	0.015	75	45	30	95
	40	1.20	20	0.021			40	116
	60	2.65	30	0.030			50	138

Trichloroethylene		Ethyl acetate		Benzene		Toluene	
°C	%	°C	%	°C	%	°C	%
0	0.07	20 ~ 40	20	7.8	20	8.5	
20	0.12			30	10.0		
40	0.26			40	12.5		
60	0.67			50	16.0		
80	1.50						
86	1.76						

Xylene		TNT	
°C	%	°C	%
20	3.3	80	82
30	4.4	100	149
40	5.4	120	645
50	6.0		

Crude Tetryl is washed with water then recryst. from benzene or acetone^[21],
80 mg/L H₂O^[45], aqueous solubility = 80 mg/L @ 25 °C^[64], 75 mg/L H₂O @ 25 °C^[71]

g Tetryl/100 *g* solvent @ various temperatures^[21]:

Solvent	@ 20 °C	@ 50 °C	@ 60 °C	@ 70 °C
Water	0.0075	0.0195	0.035	0.066
EtOH (95% vol.)	0.563	1.72	2.64	5.33
CCl ₄	0.025	0.095	0.154	0.297
CHCl ₃	0.57	1.78	2.65	—
Ethylene chloride	3.8	12.0	18.8	45.0
CS ₂	0.021	—	—	—
Et ₂ O	0.418	—	—	—

Solubility of Tetryl (g) in 100 g solvent^[48]:

$T(^{\circ}\text{C})$	H ₂ O	95% Alcohol	CCl ₄	CHCl ₃	CS ₂	Et ₂ O
0	0.0050	0.320	0.007	0.28	0.0090	0.188
5	0.0058	0.366	0.011	0.33	0.0120	0.273
10	0.0065	0.425	0.015	0.39	0.01246	0.330
15	0.0072	0.496	0.020	0.47	0.0177	0.377
20	0.0075	0.563	0.025	0.57	0.0208	0.418
25	0.0080	0.65	0.031	0.68	0.0244	0.457
30	0.0085	0.76	0.039	0.79	0.0296	0.493
35	0.0094	0.91	0.048	0.97	0.0392	—
40	0.0110	1.12	0.058	1.20	0.0557	—
45	0.0140	1.38	0.073	1.47	0.0940	—
50	0.0195	1.72	0.095	1.78	—	—
55	0.0270	2.13	0.124	2.23	—	—
60	0.0350	2.64	0.154	2.65	—	—
65	0.0440	3.33	0.193	—	—	—
70	0.0535	4.23	0.241	—	—	—
75	0.0663	5.33	0.297	—	—	—
80	0.0810	—	—	—	—	—
85	0.0980	—	—	—	—	—
90	0.1220	—	—	—	—	—
95	0.1518	—	—	—	—	—
100	0.1842	—	—	—	—	—

Very soluble in acetone^[66], slightly soluble in EtOH and benzene^[66], practically insoluble in water, CCl₄, Et₂O, CS₂ and trichloroethylene^[69], slightly soluble in hot EtOH and CHCl₃^[69], readily soluble in acetone, ethyl acetate, benzene, toluene, xylene and ethylene dichloride^[69], readily soluble in conc. nitric acid^[19], moderately soluble in other mineral acids^[19], forms eutectic mixture with 76.5% trinitro-*m*-xylene^[19], forms eutectic mixture with 29.5% trinitroanisole^[19]

Data from^[19]:

Solvent	g Tetryl/100 g solvent											
	0 °C	10 °C	20 °C	30 °C	40 °C	50 °C	60 °C	70 °C	80 °C	90 °C	100 °C	120 °C
Water	0.0050		0.0075		0.0110				0.810		0.184	
CCl ₄	0.007		0.015		0.058		0.154					
Et ₂ O	0.188	0.330	0.418	0.493								
95% EtOH	0.320	0.425	0.563	0.76		1.72		5.33 @ 75 °C				
CHCl ₃	0.28		0.39		1.20		2.65					
CS ₂	0.009	0.015	0.021	0.030								
Ethylene dichloride			4.5 @ 25 °C					45 @ 75 °C				
Acetone			75	95	116	138						
Trichloroethylene	0.007		0.12		0.26				1.50	1.76 @ 86 °C		
Ethyl acetate			40 approx.									
Toluene			8.4									
Xylene			3.3	4.4	5.4	6.0						
TNT									82		149	165

Super-solubility values for Tetryl in benzene (more Tetryl is soluble in benzene if a benzene soln. with solid Tetryl present is cooled to a specific temperature rather than a benzene soln. of Tetryl with solid Tetryl present is heated to the same specific temperature)^[19]:

$T(^{\circ}\text{C})$	Supersolubility (g Tetryl/100 g benzene)	Subsolubility (g Tetryl/100 g benzene)
15	10.2	3.9
25	12.2	5.5
35	14.9	7.4
45	18.25	9.7
55	22.5	13.25

Very slightly soluble in water: 0.019% @ 50 °C and 0.184% @ 100 °C^[75]

Solubility data from^[75]:

$T(^{\circ}\text{C})$	g Tetryl dissolving in 100 cm ³ of solvent							
	Water	Benzene	Acetone	Dichloroethane	Alcohol	CCl ₄	Ether	CS ₂
0	0.005	3.45		1.5	0.32	0.007	0.188	0.009
17	0.007				0.49	0.020		0.017
20	0.008	9.99	45.82	3.8	0.56	0.025	0.418	0.021
30	0.008				0.76	0.039	0.493	0.029
40	0.011			7.7	1.12	0.058		0.056
45	0.014				1.38	0.073		0.094
50	0.019		111.85		1.72	0.095		
60	0.035			18.8	2.64	0.154		
70	0.053	2.86			4.23	0.241		
75	0.066				5.33	0.297		
80	0.081	42.43		64.5				
100	0.184							

Hygroscopicity 0.04% @ 30 °C with 90% RH^[14], slightly hygroscopic^[9, 66], nonhygroscopic^[75]

Photosensitivity Aqueous solns. photolyzed almost completely within 20 days in sunlight^[64], turns yellow color when exposed to sunlight^[66], colorless (highly purified) but rapidly becomes yellow when exposed to light^[69]

Radiation sensitivity

Fairly resistant to dec. by γ -radiation^[19], sample exposure to 1.4×10^7 R passed 120 °C VST^[19], sample exposed to 1.2×10^8 R passed 100 °C VST but failed 120 °C VST^[19]; increase in mass loss on increasing exposure from 1.3×10^8 R to $\times 10^9$ R^[19], IS, VoD and explosion T only minimally affected by exposure to γ -radiation^[19], exposure to $\times 10^4$ Curie Co⁶⁰ source (γ -rays emitted @ 1.173 and 1.332 million eV) produces unreliable results^[19]

Effects of reactor irradiation, ^aaverage reactor exposure rates: fast neutrons $\phi > 0.18$ MeV 1.4×10^{13} n/cm² s, thermal neutron $\phi > 0.17$ eV 8.6×10^{13} n/cm² s, gamma 4.0×10^8 R/h (3.38×10^{10} ergs/g(C)(h gamma)^[89]:

Irradia- tion time (min)	Total neutron dose		Total gamma (R)	Weight loss (%)	10% loss on TGA (°C)	150° avg. gas evolu- tion (ml/g/h)	DTA peak exo- therm @ 20 °C/ min (°C)	5 s explo- sion T (°C)
	Fast (n/ cm ²)	Thermal (n/cm ²)						
0								
25	2.2×10^{16}	1.2×10^{17}	1.9×10^8	2.14				
125	10.0×10^{16}		8.8×10^8			Sample ignited		

Tetryl irradiated at ambient T using 0.41 MeV ¹⁹⁸₇₉Au γ -rays; volumes of gas produced measured during and after irradiation, amount of gas evolved as function of gamma dose^[89]:

$\times 10^7$ R	Gas evolved (ml/g) @ STP
1	< 0.1
2	0.1
3	2
4	3
5	0.5
6	0.6
7	0.8
8	1.0
9	1.4

Data obtained from explosives after exposure to gamma radiation^[76]:

Weight of sample (g)	5
Vol. of gas produced (ml/g) in following times (days)	
10	0.10
20	0.20
30	0.35
40	0.48
50	0.66
90	1.40
Total irradiation time (days)	90
Melting points, corrected (°C)	
Original material	128.8
Irradiated material	127.8
IS (B.M. apparatus) (cm)*	
Original material	25
Irradiated material	26
Sand test, 200 g bomb, <i>g</i> of sand crushed when sample was initiated by 0.30 g LA	
Original material	56.4
Irradiated material	56.0

Data from^[93]:

Exposure rate (R/h)	Total dose (R)	Vacuum stability test		
		100 °C (cc/g/40 h)	120 °C (cc/g/40 h)	200 °C (cc/.2 g/2 h)
8.5×10^5	Control		2.39	Deflagrated (8 min)
	1.4×10^7	0.45	5.77	Deflagrated (3 min)
	1.2×10^8	3.08	11 + (16 h)	Deflagrated (3 min)
	1.0×10^9	11 + (10 h), 6.98		

DTA for irradiated explosives @ 20 °C/min^[93]:

Total dose (R)	Endotherms				Exotherms			
	First		Second		First		Second	
	Onset (°C)	Peak (°C)	Onset (°C)	Peak (°C)	Onset (°C)	Peak (°C)	Onset (°C)	Peak (°C)
0	120	128			157	220	230	268
1.4×10^7	120	128			173	219	235	270
1.2×10^8	120	127			145	220	230	270
1.05×10^9	93	117			145	195	199	210
1.44×10^9	75	109			150	164	170	203

TGA for irradiated explosives^[93]:

Total dose (R)	Heating rate (°C/min)	Weight (mg)	Start of dec (°C)	10% weight loss T (°C)	Total weight loss (%)	Remarks
0	20	9.8	180	–	7 @ 215 °C	Detonated @ 214 °C
1.4×10^7	20	9.7	180	–	8 @ 216 °C	Detonated @ 216 °C
1.2×10^8	20	10.0	140	–	7 @ 212 °C	Detonated @ 212 °C

Effect of gamma radiation on the mpt. and color^[93]:

Total dose (R)	mpt. (°C)	Color
0	129	Yellow
1.4×10^7	129	Dark yellow
1.2×10^8	128	Brownish yellow
1.0×10^9		Brownish yellow

	IS for irradiated explosives, 50% fire height in inches, Bruceton method (P.A. apparatus, 2 kg mass) ^[93] :				
	Total Co ⁶⁰ gamma dose (R)		\bar{X} mean (in)	σ std. dev. (in)	
	0		17.3	0.96	
	1.4×10^7		16.2	0.81	
	1.2×10^8		19.5	0.86	
	1.0×10^9		18.25	3.28	
	Effect of gamma radiation on explosion T (5 s explosion T in °C) and activation energy (kcal/mol) ^[93] :				
	Total dose (R)		5 s explosion T (°C)	Apparent activation energy (kcal/mol)	
	0		243	14.18	
	1.2×10^8		236	13.52	
	Effect of gamma radiation on rates of detonation ^[93] :				
	Total dose (R)	Density (g/cc)	Density after irradiation (g/cc)	Rate of detonation (m/s)	Detonation pressure (kbar)
0	1.69	—	7,540	240	
1.1×10^7	1.69	1.69	7,515	239	
1.3×10^8	1.65	1.62	7,400	222	
1.0×10^9	1.62	1.47	7,010	181	
Compatibility	Hydrolyzed by boiling aqueous sodium carbonate ^[48] , turns gray when graphite added as lubricant ^[66] , not adversely affected by moisture ^[66] , corrodes steel when wet or dry ^[66] , reacts slightly with iron, zinc and brass in presence of moisture ^[66] , slight corrosion of steel and zinc in presence of 0.5% moisture but no significant effect on other metals ^[69] , no effect on metals coated with acid-proof black paint, baked oil, NRC compound or Shellac ^[69] , highly resistant to attack by dil. mineral acids ^[19] , reacts with concentrated or weak basic solns. ^[19] , no dec. on prolonged boiling in sulfuric acid ^[19] , reacts with aniline in benzene soln. @ RT ^[19] , compatible with many glues/resins (e.g., Adhesive EC 1099, Dapon resin, Delrin, Epoxy 907, Galvanoplast, conductive paint, Glastimat No. 1, Lexan, Loctite 404, Molyube No.				

18, Permacel tape, Polyesters, polysulfide rubber sealant, polyurethane vulcanizing rubbers, Silastic, Silicones and urea formaldehyde as well as Adiprene and Eastman adhesives)^[19], heavily corrodes steel^[19], slightly corrodes Fe, Zn, Zn plated steel, Sn plated steel, parkerized steel, brass and Monel^[19], Tetryl does not corrode Cu, Sn, bronze, Ni, Pb, Cu plated steel, stainless steel, Cd, Al, Ag and Ti^[19], compatible with graphite, stearic acid or magnesium stearate and black powder^[19], does not react with metals^[9], does not react with metals^[75], reacts with alkalis, Na₂CO₃ and K₂CO₃^[75], slow dec. on heating in water^[75]

A = no reaction, B = slight reaction, C = reacts readily, D = reacts to form sensitive materials, H = heavy corrosion of metals, VS = very slight corrosion of metals, S = slight corrosion of metals, N = no corrosion, data from^[76].

Aluminum	A	N
Zinc	B	VS
Iron	B	S
Steel	C	H
Tin	A	N
Cadmium	A	
Copper	A	N
Nickel	A	N
Lead	A	N
Cadmium plated steel	A	N
Copper plated steel	A	VS
Nickel plated steel	A	N
Zinc plated steel	A	N
Tin plated steel	B	VS
Brass	B	VS
Bronze	A	VS
18–8 stainless steel	A	N
Titanium		N
Silver		N

Wedge test [mm]	0.26 mm (LANL) ^[47]		
	Data from ^[21] :		
	Density (g/cm ³)	Distance, x^* and time t^* to detonation (mm and μ s)	Pressure range (GPa)
	1.70	$\log P = (0.79 \pm 0.01) - (0.42 \pm 0.01) \log x^*$ $\log P = (0.55 \pm 0.01) - (0.39 \pm 0.01) \log t^*$	$2.22 < P < 8.53$
	1.60	$\log P = (0.73 \pm 0.01) - (0.65 \pm 0.01) \log x^*$ $\log P = (0.4 \pm 0.01) - (0.55 \pm 0.01) \log t^*$	$1.08 < P < 8.02$
	1.50	$\log P = (0.75 \pm 0.01) - (0.81 \pm 0.01) \log x^*$ $\log P = (0.35 \pm 0.01) - (0.64 \pm 0.01) \log t^*$	$0.62 < P < 7.09$
	1.40	$\log P = (0.84 \pm 0.01) - (0.99 \pm 0.02) \log x^*$ $\log P = (0.35 \pm 0.01) - (0.75 \pm 0.01) \log t^*$	$0.51 < P < 6.84$
	1.30	$\log P = (0.87 \pm 0.05) - (1.11 \pm 0.07) \log x^*$ $\log P = (0.33 \pm 0.02) - (0.83 \pm 0.03) \log t^*$	$0.37 < P < 86.91$
where P = pressure in GPa			
Minimum priming charge test [mg]	$W_{50} = 1.5$ mg XTX 8003 @ 1.682 g cm^{-3} ^[21] , 2 mg (LANL) ^[47]		
Bullet test [f/s]	2,130 (LANL) ^[47]		
Rifle bullet test	More sensitive than TNT ^[19, 69] , easily detonated by penetration of a rifle bullet ^[9]		
Rifle bullet impact test	13% explosions, 54% partials, 10% burned and 23% unaffected in trials ^[14, 76]		
Thermal conductivity [W°C ⁻¹ m ⁻¹]	$5.81 \times 10^{-4} \text{ cal/s/cm/}^\circ\text{C}$ @ 1.394 g cm^{-3} ^[14] , $6.83 \times 10^{-4} \text{ cal/s/cm/}^\circ\text{C}$ @ 1.528 g cm^{-3} ^[14] , $6.83 \times 10^{-4} \text{ cal/s/cm/}^\circ\text{C}$ (@ 1.53 g cm^{-3}) ^[19, 21] , $5.81 \times 10^{-4} \text{ cal/s/cm/}^\circ\text{C}$ (@ 1.39 g cm^{-3}) ^[21]		
	Obtained using MDSC apparatus (modulated DSC) ^[52] :		
	T (°C)	K (W°C ⁻¹ m ⁻¹) (nonisothermal)	K (W°C ⁻¹ m ⁻¹) (isothermal)
	-3	0.171	0.186
	17	0.165 (0.084–0.286, nonisothermal, lit. value)	0.186 (0.084–0.286, isothermal, lit. value)
	47	0.154	0.189

Specific heat capacity [J/g °C]	Values from ^[14] : <table><tr><td>T (°C)</td><td colspan="2">Specific heat (cal/g/°C)</td></tr><tr><td>−100</td><td colspan="2">0.182</td></tr><tr><td>−50</td><td colspan="2">0.200</td></tr><tr><td>0</td><td colspan="2">0.212</td></tr><tr><td>50</td><td colspan="2">0.223</td></tr><tr><td>100</td><td colspan="2">0.236</td></tr></table> Values from ^[52] : <table><tr><td>T (°C)</td><td>C_p (J/g°C) (Nonisothermal)</td><td>C_p (J/g°C) (isothermal)</td></tr><tr><td>−3</td><td>0.812</td><td>0.80</td></tr><tr><td>+17</td><td>0.863</td><td>0.844</td></tr><tr><td>+47</td><td>0.939</td><td>0.910</td></tr></table> 0.218 kcal/g°C @ 20 °C ^[75] , C _p ²⁹⁸ = 72.2 cal mol ^{−1} K ^{−1} ^[84] , 0.211 + 2.6 × 10 ^{−4} T cal/g-°C @ −100< T<100 °C (heat capacity @ constant pressure) ^[21]			T (°C)	Specific heat (cal/g/°C)		−100	0.182		−50	0.200		0	0.212		50	0.223		100	0.236		T (°C)	C _p (J/g°C) (Nonisothermal)	C _p (J/g°C) (isothermal)	−3	0.812	0.80	+17	0.863	0.844	+47	0.939	0.910
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+17	0.863	0.844																															
+47	0.939	0.910																															
Bourdon manometer	0.81 mL/g @ 120 °C, 48 h ^[61]																																
ARC [min]	Isothermal ARC data for depth charge Tetryl, 1 g sample, @ 135 °C ^[62] : <table><tr><td>Tetryl sample</td><td colspan="2">Time to noticeable dec. (min)</td></tr><tr><td>As-received, recrystallized Tetryl</td><td colspan="2">159 (lowest), 241 (highest)</td></tr><tr><td>As-received depth-charge</td><td colspan="2">159, 141</td></tr><tr><td>Highly aged depth-charge Tetryl (15 days @ 115 °C)</td><td colspan="2">127, 150</td></tr></table>			Tetryl sample	Time to noticeable dec. (min)		As-received, recrystallized Tetryl	159 (lowest), 241 (highest)		As-received depth-charge	159, 141		Highly aged depth-charge Tetryl (15 days @ 115 °C)	127, 150																			
Tetryl sample	Time to noticeable dec. (min)																																
As-received, recrystallized Tetryl	159 (lowest), 241 (highest)																																
As-received depth-charge	159, 141																																
Highly aged depth-charge Tetryl (15 days @ 115 °C)	127, 150																																
Heat of fusion [cal/g]	22.2 ^[14] , 5.9 kcal/mol ^[19] , 22.2 (latent heat of melting) ^[21] , 21.6 ^[64] , ΔH _{melt} = 5.48 ± 0.09 kcal/mol ^[84] , ΔH _{melt} = 6.18 ± 0.07 kcal/mol ^[84] , ΔH _{melt} = 5.9 kcal/mol ^[84]																																
Heat of vaporization [kcal/mol]	26 ^[19]																																
Diffusion coefficient [cm ² /s]	0.059 (air) ^[64] , 5.99 × 10 ^{−6} (water) ^[64]																																
Coefficient of thermal expansion	0.32 × 10 ^{−3} per degree ^[19]																																
Log K _{ow}	1.65 ^[64] , 2.04 ^[71]																																

Log K_{oc}	1.69 ^[64]																								
Biodegradation	Very slow hydrolysis with extrapolated $t_{1/2} = \sim 302 \pm 76$ days @ 20 °C, pH 6.8 ^[64]																								
Plate dent test	Method A, pressed, confined, $\rho = 1.50 \text{ g cm}^{-3}$, brisance = 116% TNT ^[14] , method B, pressed, not confined, $\rho = 1.59 \text{ g cm}^{-3}$, brisance = 115% TNT ^[14] , Method B, pressed, not confined, $\rho = 1.36 \text{ g cm}^{-3}$, brisance = 96% TNT ^[14] , 115% TNT ^[19] , charge diameter = 41.3 mm, $\rho = 1.681 \text{ g cm}^{-3}$, dent depth = 8.10 mm, charge height = 203 mm ^[21]																								
Booster sensitivity test	100 g Tetryl, 2.01 in wax for 50% detonation, $\rho = 1.58 \text{ g cm}^{-3}$ ^[14, 76] , pressed Tetryl, $\rho = 1.58 \text{ g cm}^{-3}$, 50% Gap = 2.01 in ^[76]																								
Fragmentation tests	<p>Data from^[14]:</p> <table border="1"> <tr><td colspan="2">90 mmHE, M71 projectile, lot WC-91:</td></tr> <tr><td>Density (g/cc)</td><td>1.58</td></tr> <tr><td>Charge wt. (lb)</td><td>2.052</td></tr> <tr><td colspan="2">Total no. of fragments:</td></tr> <tr><td>For TNT</td><td>703</td></tr> <tr><td>For Tetryl</td><td>864</td></tr> <tr><td colspan="2">3 in HE, M42A1 projectile, lot KC-5</td></tr> <tr><td>Density (g/cc)</td><td>1.62</td></tr> <tr><td>Charge wt. (lb)</td><td>0.848</td></tr> <tr><td colspan="2">Total no. of fragments:</td></tr> <tr><td>For TNT</td><td>514</td></tr> <tr><td>For Tetryl</td><td>605</td></tr> </table> <p>121% TNT^[19]</p>	90 mmHE, M71 projectile, lot WC-91:		Density (g/cc)	1.58	Charge wt. (lb)	2.052	Total no. of fragments:		For TNT	703	For Tetryl	864	3 in HE, M42A1 projectile, lot KC-5		Density (g/cc)	1.62	Charge wt. (lb)	0.848	Total no. of fragments:		For TNT	514	For Tetryl	605
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Hardness	<1 (Moh's scale, scratch hardness) ^[19]																								
Refractive index	1.546 (α) ^[19] , 1.632 (β) ^[19] , 1.74 (γ) ^[19]																								
Dielectric constant	<p>Values from^[19]:</p> <table border="1"> <tr> <th>Density (g/cc)</th><th>Dielectric constant measured at 35 giga cycles</th></tr> <tr><td>0.9</td><td>2.059</td></tr> <tr><td>1.0</td><td>2.163</td></tr> <tr><td>1.4</td><td>2.782</td></tr> <tr><td>1.5</td><td>2.905</td></tr> <tr><td>1.6</td><td>3.097</td></tr> <tr><td>1.7</td><td>3.304</td></tr> </table>	Density (g/cc)	Dielectric constant measured at 35 giga cycles	0.9	2.059	1.0	2.163	1.4	2.782	1.5	2.905	1.6	3.097	1.7	3.304										
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1.4	2.782																								
1.5	2.905																								
1.6	3.097																								
1.7	3.304																								

Laser ignition	No ignition on direct exposure to laser beam ^[19] , ignition observed if Tetryl ($\rho = 1.08 \text{ g cm}^{-3}$) is coated with thin metal film ^[19] , no initiation observed if Tetryl ($\rho \approx 1.08 \text{ g cm}^{-3}$) is coated with thin metal film ^[19] , successful detonation if Tetryl sample compressed against glass plate (Ruby laser (6,943 Å) both in free running and Q-switch modes) ^[76]																							
Copper cylinder compression test	117–125% TNT ^[19]																							
Lead block compression test	112% TNT ^[19]																							
USA Small-Scale Cookoff Bomb test (SCB test)	Pressed Tetryl, heater voltage = 110, cookoff temperature = 215 °C, cookoff time = 14.5 min, cookoff reaction = detonation ^[73]																							
Heat of decomposition [cal/g]	191 (est.) ^[74]																							
Flash point [°C]	190 ^[75]																							
Hess brisance	19 mm ^[75]																							
Critical air gap	0.184 in (0.2 in diameter) ^[76]																							
Critical Lucite gap	50% gap = 0.434 in, DBg = 3.63 (donor = RDX, 1 in long, 0.2 in diameter, pressed in steel @ 10 kpsi) ^[76]																							
100 kg drop test	10% firing, 2.8 ft height, cast $\rho = 1.57 \text{ g cm}^{-3}$ (cast), partially exploded ^[76]																							
Laser sensitivity	<div>Examples of heat/shock reactions in experimental detonation systems; detonation conditions using laser-produced heat and shock^[77]:</div> <table><tr><th>Density or pressing force</th><th>Detonator type</th><th>Nominal wave-length (nm)</th><th>Spot diameter (microns)</th><th>Power or energy (J)</th><th>Function time (ms)</th><th>Laser type</th><th>Pulse duration (ms)</th></tr><tr><td>1.08 g/cc</td><td>Confined</td><td>694</td><td>< 3,000</td><td>4</td><td>5.58</td><td>Q-switched ruby</td><td>1.45</td></tr></table>								Density or pressing force	Detonator type	Nominal wave-length (nm)	Spot diameter (microns)	Power or energy (J)	Function time (ms)	Laser type	Pulse duration (ms)	1.08 g/cc	Confined	694	< 3,000	4	5.58	Q-switched ruby	1.45
Density or pressing force	Detonator type	Nominal wave-length (nm)	Spot diameter (microns)	Power or energy (J)	Function time (ms)	Laser type	Pulse duration (ms)																	
1.08 g/cc	Confined	694	< 3,000	4	5.58	Q-switched ruby	1.45																	
Combustion T [K]	Burn rate and equilibrium combustion temperature ^[78] : $T_e = 2,775 \text{ K}$ ^[78] , $m = 1.55 \text{ g cm}^{-2} \text{ s}^{-1}$ (100 atm.) ^[78]																							
Detonation failure thickness	$L_{95} = 0.079 \text{ mm}$, failure thickness = 0.267 mm @ 1.684 g cm^{-3} ^[21]																							

Manometric bomb	4,684 kg/cm ² (@ 0.3 g cm ⁻³ , manometric bomb) ^[48] , 2,423 kg/cm ² (@ 0.20 g cm ⁻³ , manometric bomb) ^[48] , 3,243 kg/cm ² (@ 0.25 g cm ⁻³ , manometric bomb) ^[48]
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	Tetryl ^{[19, 20, 38]†}	Tetryl ^[21]
Chemical formula	C ₇ H ₅ N ₅ O ₈	C ₇ H ₅ N ₅ O ₈
Molecular weight [g mol ⁻¹]	287.14	287.14
Crystal system	Monoclinic	Monoclinic
Space group	<i>P</i> 2 ₁ / <i>c</i> (no. 14)	
<i>a</i> [Å]	14.1290 ± 0.0019	14.129
<i>b</i> [Å]	7.3745 ± 0.0013	7.374
<i>c</i> [Å]	10.6140 ± 0.0020	10.614
α [°]	90	90
β [°]	95.071 ± 0.017	95.07
γ [°]	90	90
<i>V</i> [Å ³]		
<i>Z</i>	4	4
ρ_{calc} [g cm ⁻³]	1.731	
<i>T</i> [K]	295	

† Tetryl forms the solid crystalline hydrate C₇H₅N₅O₈•¹/₄ H₂O when H₂O is added to an acetone soln. of Tetryl^[38]

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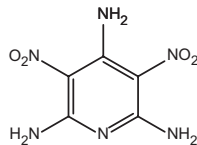
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2,4,6-Triamino-3,5-dinitropyridine

Name [German, acronym]: Triaminodinitropyridine [2,4,6-triamino-3,5-dinitropyridin, TADNP]

Main (potential) use: Possible thermally stable explosive^[1]

Structural formula:



	TADNP		
Formula	C ₅ H ₆ N ₆ O ₄		
Molecular mass [g mol ⁻¹]	214.14		
Appearance at RT			
IS [J]			
FS [N]			
ESD [J]			
N [%]	39.25		
Ω(CO ₂) [%]	-67.25		
T _{m,p.} [°C]			
T _{b,p.} [°C]			
T _{phase transition} [°C]			
T _{dec.} [°C]			
ρ [g cm ⁻³]	1.82		
Heat of formation	-38.9 kJ/mol		
Heat of combustion			
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
-Δ _{ex} U° [kJ kg ⁻¹]	3493		
T _{ex} [K]	2555		

p_{C-J} [kbar]	224		
VoD [$m\ s^{-1}$]	7749		
V_0 [$L\ kg^{-1}$]	725		

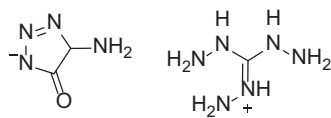
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Triaminoguanidinium 1-aminotetrazol-5-oneate

Name [German, acronym]: Triaminoguanidinium 1-aminotetrazol-5-oneate
[ATO-TAG]

Main (potential) use: Secondary (high) explosive

Structural formula:



	ATO · TAG		
Formula	C ₂ H ₁₁ N ₁₁ O		
Molecular mass [g mol ⁻¹]	205.22		
Appearance at RT	Yellow powder ^[1]		
IS [J]	>40 ^[1]		
N [%]	75.09		
Ω(CO ₂) [%]	-50.73		
T _{m.p.} [°C]	154.5 (DSC-TG @ 10 °C/min) ^[1]		
T _{dec.} [°C]	214.5 (DSC-TG @ 10 °C/min) ^[1]		
ρ [g cm ⁻³]	1.569 (@ 296 K) ^[1]		
Heat of formation	743.27 kJ/mol (ΔH _f ^o) ^[1] , 3,622 kJ/kg (ΔH _f ^o) ^[1]		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
-Δ _{ex} U ^o [kJ kg ⁻¹]	5,343		
T _{ex} [K]	3,025		
p _{C-J} [GPa]	31.8	31.0 (calcd., K-J) ^[1]	
VoD [m s ⁻¹]	9,492 (@ 1.509 g cm ⁻³ , Δ _f H = 743.27 kJ mol ⁻¹)	8,720 (calcd., K-J) ^[1]	
V ₀ [L kg ⁻¹]	977		

	ATO-TAG^[1]
Chemical formula	C ₂ H ₁₁ N ₁₁ O
Molecular weight [g mol ⁻¹]	205.22
Crystal system	Orthorhombic
Space group	<i>Pbca</i> (no. 61)
<i>a</i> [Å]	12.8237(6)
<i>b</i> [Å]	6.7049(3)
<i>c</i> [Å]	20.2018(10)
α [°]	90
β [°]	90
γ [°]	90
<i>V</i> [Å ³]	1,736.98(14)
<i>Z</i>	8
ρ_{calc} [g cm ⁻³]	1.569
<i>T</i> [K]	296

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VoD [m s ⁻¹]	8,796 ^[3]		
V ₀ [L kg ⁻¹]	932 ^[3]		
Solubility [g/mL]	Recryst. from hot EtOH ^[3]		
Koenen test	≥10 mm (hole width of steel sleeve) ^[3]		

	TAGDN ^[2, 3]
Chemical formula	CH ₉ N ₉ O ₄
Molecular weight [g mol ⁻¹]	211.17
Crystal system	Orthorhombic
Space group	<i>Pbca</i> (61)
<i>a</i> [Å]	12.5217(3)
<i>b</i> [Å]	8.1036(2)
<i>c</i> [Å]	16.9859(4)
α [°]	90
β [°]	90
γ [°]	90
<i>V</i> [Å ³]	1,723.57(7)
<i>Z</i>	8
ρ_{calc} [g cm ⁻³]	1.628
<i>T</i> [K]	100
	Recryst. from hot EtOH ^[3]

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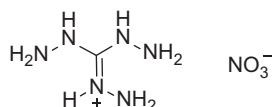
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Triaminoguanidinium nitrate

Name [German, acronym]: Triaminoguanidine nitrate [triaminoguanidinnitrat, TAGN]

Main (potential) use: Ingredient for LOVA gun propellants^[6], ingredient in some gun propellants^[15], often added to RDX propellant formulations to increase the burning rate and particularly important in LOVA propellant formulations^[17, 19], can be added to solid propellant to increase its burning rate^[18], gas generators^[19], tested as a component of gun propellants with nitramines, organic nitric acid esters and polymeric binders^[20], as an additive to double-base propellants or as a dual-system with azidopolymers^[20], possible future component of gas-generator systems^[20]

Structural formula:



	TAGN
Formula	CH ₉ N ₇ O ₃
Molecular mass [g mol ⁻¹]	167.10
Appearance at RT	colorless crystals/white powder ^[15] , colorless crystals ^[17] , pink discoloration indicates impurity ^[19]
IS [J]	4 Nm ^[6, 20] , 23 cm (ERL, type 12) ^[7] , 11 in (2 kg mass, P.A.) ^[8] , 5.5 Nm ^[10] , 13 Nm (75% TAGN, 10% PU, 15% TA)* ^[20] , 6.5 Nm (80% TAGN, 10% CA, 10% TA)* ^[20]
FS [N]	>120 ^[6] , 120 ^[20] , 216 (75% TAGN, 10% PU, 15% TA)* ^[20] , 216 (80% TAGN, 10% CA, 10% TA)* ^[20]
ESD [J]	Spark test (3 mil foil) >1.0 ^[7]
N [%]	58.67
Ω(CO ₂) [%]	−33.5
T _{phase transition} [°C]	LT (−10 °C) polymorph is <i>Pbca</i> and RT polymorph is <i>Pbcm</i> ^[16] , −28.4 (endo, onset), −10.0 (endo, peak max) (DSC @ 20 °C/min, ΔH = 0.483 kJ/mol, second order) ^[17, 18]
T _{m.p.} [°C]	216–220 ^[1] , 216 ^[6, 8] , 215 (endo, DTA, nonreactive quartz sample containers, @ 5–30 °C/min) ^[11] , 215 ^[14]

$T_{\text{glass transition}} [^{\circ}\text{C}]$	−65 (75% TAGN, 10% PU, 15% TA)* ^[20]		
$T_{\text{dec.}} [^{\circ}\text{C}]$	221 (DSC @ 4 °C/min) ^[1] , 257 (DSC @ 64 °C/min) ^[1] , 235 (exotherm, DTA) ^[10] , TG, nonreactive quartz sample container, @ 5–30 °C/min: 3 stage weight loss process; stage 1 = 0% weight loss @ 215 °C and 27% weight loss @ 225 °C; stage 2 = between 27% weight loss @ 225 °C and 92% weight loss @ 300 °C; stage 3 = 92% (@ 300 °C)–100% (@ 550 °C) weight loss ^[11] , dec. begins immediately after the mpt. and reaches a maximum @ ~ 232 °C (DSC @ 10 °C/min) ^[19]		
$\rho [\text{g cm}^{-3}]$	1.5 ^[6, 20] , 1.594 (@ 293 K) ^[2] , 1.536, 1.630 (measured crystals) ^[9] , 1.54 ^[14] , 1.59 ^[15]		
Heat of formation	−287.9 kJ/kg (enthalpy of form., ICT thermochemical code) ^[3, 6] , −69 cal/g ^[4] , −72.0 kcal/kg (enthalpy of form.) ^[12] , −12.01 kcal/mol ($\Delta H^{\circ}_{\text{f}}$, exptl.) ^[13] , −11.42 kcal/mol ($\Delta H^{\circ}_{\text{f}}$, calcd.) ^[13] , −68.8 kcal/kg (ΔH_{f}) ^[14] , 11.71 kcal/mol (Q_{f}) ^[8] , −280 J/g (ΔH_{f}) ^[11] , −11.5 kcal/mol (ΔH_{f} (s), @ 298 K, bomb calorimetry) ^[7] , −48.1 kJ/mol (enthalpy of form.) ^[15] , −280 kJ/kg ^[20] , −48.1 kJ/mol (enthalpy of form., exptl.) ^[21] , −35.2 kJ/mol (enthalpy of form., calcd., emp.) ^[21] , −69.2 kJ/mol (enthalpy of form., calcd., S-D method) ^[21]		
Heat of combustion	2,334 cal/g (Q_{c}) ^[8]		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^{\circ} [\text{kJ kg}^{-1}]$	4,237	3,974 (calcd., ICT-code) ^[3] 943 kcal/kg (@ 1.570 g cm ^{−3} , calcd.) [H ₂ O vapor] ^[12]	3,974 [H ₂ O (l)] ^[6] 3,492 [H ₂ O (g)] ^[6] 920.98 cal/g ^[8] 944 kcal/kg (@ 1.570 g cm ^{−3}) [H ₂ O vapor] ^[12] 3,490 [H ₂ O (g)] ^[15]
$T_{\text{ex}} [\text{K}]$	2,707	2,593 (calcd., ICT-code) ^[3]	
$p_{\text{C-J}} [\text{kbar}]$	279	132.1 MPa (calcd., ICT-code) ^[3]	
VoD [m s ^{−1}]	8,893 (@ TMD)	8,048 (@ 1.47 g cm ^{−3}) ^[10]	5,300 (@ 0.95 g cm ^{−3}) ^[6, 15] 7,930 (@ 1.46 g/cc) ^[8] 5,350 (@ 1.00 g cm ^{−3}) ^[8]
$V_0 [\text{L kg}^{-1}]$	1,034		1,163 ^[5, 6] 1,206 ^[8]

Trauzl test [cm ³ , % TNT]	350 cc (10 g sample) ^[8]
Sand test [g]	34.9 g sand crushed (200 g bomb) ^[8]
Gap test	18 kbar, charge $\rho = 1.49 \text{ g cm}^{-3}$ ^[10] , 0 mm H ₂ O column (75% TAGN, 10% PU, 15% TA)* ^[20]
5 s explosion T [°C] Explosion T [°C] Deflagration T [°C] Autoignition T [°C]	225 (DTA/TG @ 6 °C/min) ^[10] , 260 ^[8] 227 ^[8, 19] , 277 ^[20] 238 (75% TAGN, 10% PU, 16% TA @ 20 °C/min)* ^[20] , 237 (80% TAGN, 10% CA, 10% TA, @ 20 °C/min)* ^[20]
100 °C heat test [% mass loss]	0.15% mass loss in first 48 h, 2.73% mass loss in second 48 h, no explosion in 100 h ^[8]
Vacuum stability test [cm ³ /h]	1.06 cc/g @ 120 °C ^[8] , 0.07 mL/g (40 h/100 °C, 75% TAGN, 10% PU, 16% TA @ 20 °C/min)* ^[20] , 0.32 mL/g (40 h/100 °C, 80% TAGN, 10% CA, 10% TA, @ 20 °C/min)* ^[20]
Thermal stability	Colored (usually pink) crystals are found during synthesis/storage/processing of TAGN ^[19] , propellants made from pink discolored TAGN show decrease in ballistic properties cf. propellants made from nondiscolored TAGN ^[19] , metal ion contamination should be avoided and fast solvent removal are necessary ^[19] , pink color can be removed by washing with deionized water – the pink color is suggested to be due to liquid trapped inside TAGN crystals ^[19]

Burn rate [mm/s]	Extremely fast ^[18]					
	Burning properties of TAGN gas generator formulations, data from ^{[20]*} :					
	Burning properties $r = A \cdot p^n$		75% TAGN PU/TA	80% TAGN CA/TA	70% TAGN PU/ BDNPF/A	70% TAGN GAP/ BDNPF/A
	Burn rates, r @ 7 MPa in mm/s	−30 °C	3.0	–	–	–
		+20 °C	3.5	5.1	6.1	9.2
		+50 °C	4.8	6.0	–	–
	Pressure exponent, n	−30 °C	0.42	–	–	–
		+20 °C	0.54	0.45	0.65	0.56
		+50 °C	0.59	–	–	–
	A-value	−30 °C	0.504	–	–	–
+20 °C		0.353	0.754	0.385	0.852	
+50 °C		0.391	–	–		
Data from ^{[20]*} :						
TAGN/PU-GG		TAGN-content				
		80%		75%		
Burning T , T_c		1,325 K		1,260 K		
Yield of gases, n_m		57.0 mol/kg		55.8 mol/kg		
Density, ρ		1.40 g/cm ³		1.37 g/cm ³		
Vol. yield of gases, n_n		97.8 mol/dm ³		76.7 mol/dm ³		
Burning rate @ 10 MPa		-		4.5 mm/s		
Compatibility	Metal ion contamination should be avoided and fast solvent removal are necessary ^[19] , addition of NC to propellant formulations can reduce the stability of the TAGN propellant, but addition of Ascardite (stabilizer) can minimize the loss in stability of NC/TAGN propellants ^[19]					

Heat capacity	Heat capacity is relatively constant from –100–55 °C, but increases in the temperature range –55–60 °C, DSC @ 20 °C/min, 5–10 mg sample ^[17] :																																																																														
	<table><tr><th rowspan="2">T (°C)</th><th colspan="2">Heat capacity</th></tr><tr><th>J/kg</th><th>Cal/kg</th></tr><tr><td>–70</td><td>1,326</td><td>0.315</td></tr><tr><td>–60</td><td>1,336</td><td>0.319</td></tr><tr><td>–60</td><td>1,364</td><td>0.325</td></tr><tr><td>–45</td><td>1,386</td><td>0.331</td></tr><tr><td>40</td><td>1,413</td><td>0.338</td></tr><tr><td>–35</td><td>1,441</td><td>0.344</td></tr><tr><td>–30</td><td>1,466</td><td>0.358</td></tr><tr><td>–25</td><td>1,495</td><td>0.357</td></tr><tr><td>–20</td><td>1,525</td><td>0.364</td></tr><tr><td>–15</td><td>1,543</td><td>0.369</td></tr><tr><td>–10</td><td>1,610</td><td>0.385</td></tr><tr><td>–5</td><td>1,570</td><td>0.375</td></tr><tr><td>0</td><td>1,534</td><td>0.367</td></tr><tr><td>5</td><td>1,559</td><td>0.373</td></tr><tr><td>10</td><td>1,586</td><td>0.379</td></tr><tr><td>20</td><td>1,634</td><td>0.391</td></tr><tr><td>30</td><td>1,688</td><td>0.403</td></tr><tr><td>40</td><td>1,738</td><td>0.414</td></tr><tr><td>50</td><td>1,781</td><td>0.426</td></tr><tr><td>60</td><td>1,811</td><td>0.433</td></tr><tr><td>70</td><td>1,842</td><td>0.440</td></tr><tr><td>80</td><td>1,881</td><td>0.450</td></tr><tr><td>90</td><td>1,943</td><td>0.456</td></tr><tr><td>100</td><td>1,959</td><td>0.466</td></tr></table>		T (°C)	Heat capacity		J/kg	Cal/kg	–70	1,326	0.315	–60	1,336	0.319	–60	1,364	0.325	–45	1,386	0.331	40	1,413	0.338	–35	1,441	0.344	–30	1,466	0.358	–25	1,495	0.357	–20	1,525	0.364	–15	1,543	0.369	–10	1,610	0.385	–5	1,570	0.375	0	1,534	0.367	5	1,559	0.373	10	1,586	0.379	20	1,634	0.391	30	1,688	0.403	40	1,738	0.414	50	1,781	0.426	60	1,811	0.433	70	1,842	0.440	80	1,881	0.450	90	1,943	0.456	100	1,959	0.466
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Holland test	0.04% (8–72 h/105 °C, 75% TAGN, 10% PU, 16% TA @ 20 °C/min)* ^[20] , 0.57% (8–72 h/105 °C, 80% TAGN, 10% CA, 10% TA, @ 20 °C/min)* ^[20]																																																																														

*PU, viscoelastic polyester urethane polymers; TA, triacetin; CA, thermoplastic cellulose acetate

	TAGN ^[2, 16]	TAGN ^[9]	TAGN ^[16, 17]	TAGN ^[18]	TAGN ^[18]
		(Neutron)	LT-polymorph	LT-polymorph	Above –10 °C the LT-polymorph transforms into this polymorph
Chemical formula	CH ₉ N ₇ O ₃	CH ₉ N ₇ O ₃	CH ₉ N ₇ O ₃	CH ₉ N ₇ O ₃	CH ₉ N ₇ O ₃
Molecular weight [g mol ⁻¹]	167.10	167.10	167.10	167.13	167.13
Crystal system	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic
Space group	<i>Pbcm</i>	<i>Pbcm</i>	<i>Pbca</i>	<i>Pbca</i>	<i>Pbcm</i>
<i>a</i> [Å]	8.389(7)	8.389	33.07(1)	33.058(10)	8.366(2)
<i>b</i> [Å]	12.684(8)	12.684	12.581(4)	12.573(2)	12.649(2)
<i>c</i> [Å]	6.543(5)	6.543	6.518(3)	6.541(4)	6.556(1)
α [°]	90	90	90	90	90
β [°]	90	90	90	90	90
γ [°]	90	90	90	90	90
<i>V</i> [Å ³]	696.2	696.215	2,711.8	2,718.7	
<i>Z</i>	4	4		16	4
ρ_{calc} [g cm ⁻³]	1.594	1.594		1.63	1.60
<i>T</i> [K]	295	295	–100 °C	169 (–104 °C)	23 °C

Lattice parameters as a function of temperature (^atransition temperature is close to $-10\text{ }^{\circ}\text{C}$; ^bthe a axis and volume above the transition temperature are $\frac{1}{4}$ the values given in the table below)^[17]:

$T (^{\circ})$	Parameters			
	$a (\text{\AA})$	$b (\text{\AA})$	$c (\text{\AA})$	$V (\text{\AA})$
-100	33.07(1)	12.581(4)	6.518(3)	2,711.8
-64	33.199(4)	12.594(4)	6.537(4)	2,732.2
-51	33.245(7)	12.603(3)	6.544(4)	2,741.5
-27	33.344(8)	12.622(4)	6.548(2)	2,755.5
-26	33.344(9)	12.619(4)	6.546(2)	2,754.8
-13	33.408(9)	12.635(3)	6.550(3)	2,764.8
a				
-5	33.444(9) ^b	12.641(4)	6.552(5)	2,770.0 ^b
15	33.47(1) ^b	12.659(5)	6.559(3)	2,779.0 ^b
23	8.366(2)	12.649(2)	6.556(1)	693.8

TAGN crystals are hollow cylinders and the pink color of impure TAGN is suggested to be due to liquid being trapped inside the hollow cylinders; pure TAGN is a colorless crystalline substance^[19]

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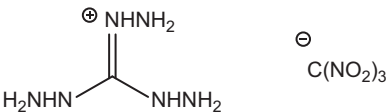
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Triaminoguanidinium nitroformate

Name [German, acronym]: Triaminoguanidinium nitroformate
[triaminoguanidiniumnitroformat, TAGNF]

Main (potential) use: academic

Structural formula:



	TAGNF		
Formula	C ₂ H ₉ N ₉ O ₆		
Molecular mass [g mol ⁻¹]	255.18		
Appearance at RT			
IS [J]	2 (BAM) ^[1]		
FS [N]	20 ^[1]		
N [%]	49.4		
Ω(CO ₂) [%]	−15.7		
T _{m.p.} [°C]	84 (DSC @ 2 °C/min) ^[1]		
T _{dec.} [°C]	105 (DSC @ 2 °C/min) ^[1]		
ρ [g cm ⁻³]	1.689 ^[1]		
Heat of formation	59.1 kcal mol ⁻¹ (Δ _f H°) ^[1]		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
−Δ _{ex} U° [kJ kg ⁻¹]	6,274 ^[1]		
T _{ex} [K]	4,358 ^[1]		
p _{C-J} [kbar]	330 ^[1]		
VoD [m s ⁻¹]	8,982 (@ 1.689 g cm ⁻³) ^[1]		
V ₀ [L kg ⁻¹]	885 ^[1]		

	TAGNF^[1]
Chemical formula	C ₂ H ₉ N ₉ O ₆
Molecular weight [g mol ⁻¹]	255.18
Crystal system	Triclinic
Space group	<i>P</i> -1 (no. 2)
<i>a</i> [Å]	8.020(2)
<i>b</i> [Å]	8.347(2)
<i>c</i> [Å]	8.515(2)
α [°]	105.49(2)
β [°]	95.03(2)
γ [°]	111.10(2)
<i>V</i> [Å ³]	501.7
<i>Z</i>	2
ρ_{calc} [g cm ⁻³]	1.689
<i>T</i> [K]	200

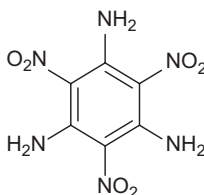
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1,3,5-Triamino-2,4,6-trinitrobenzene

Name [German, acronym]: [Triamino trinitrobenzene, triamino trinitrobenzol, TATB]

Main (potential) use: Booster in nuclear weapons^[18], plastic explosives, explosives mixture with TNT, warheads, missiles, thermoresistant insensitive explosive^[76], deep oil well exploration^[76]

Structural formula:



	TATB
Formula	$C_6H_6N_6O_6$
Molecular mass [g mol ⁻¹]	258.15
Appearance at RT	Yellow solid ^[14] , yellow solid which turns slightly green on exposure to light which then turns brown on prolonged exposure to sunlight or UV radiation ^[19] , yellow polycrystalline solid ^[20] , lemon yellow microcrystalline powder after recryst. from sulfuric acid ^[68] , fine yellow powder (average crystal size = 25–300 μm, received TATB) ^[68] , yellow crystalline solid ^[79] , pale yellow solid ^[85]
IS [J]	120.17 ^[5] , 50 Nm ^[6, 18] , 5.48 (11 in, 2 kg mass, 7 mg sample, P.A.) ^[14] , >86.8 (5 kg, 12 tool) ^[16] , >78.5 (2.5 kg, 12 tool) ^[16] , >78.5 (2.5 kg, 12B tool) ^[16] , 800 cm (50% detonations, 2.5 kg mass, ERL apparatus) ^[19] , 11 in (7 mg sample, P.A.) ^[19] , no detonation height = 200 cm (2.5 kg mass, type 12 tool, no grit, ERL apparatus) ^[19] , $H_{50} > 320$ cm (tool type 12) ^[20] , $H_{50\%} \sim 800$ cm (2.5 kg mass, type 12 tool, no grit, ERL apparatus) ^[19] , $H_{50} > 320$ cm (tool type 12B) ^[20] , $IS_{LL} = 2.0$ m ^[21] , $IS_{A50} = 10$ m ^[21] , $H_{50} \geq 111.6$ ^[24] , 22.2 in (P.A.) ^[22] , drop weight >25 Nm (BAM) ^[23] , $H_{50} \geq 100$ (5 kg mass, tool type 12) ^[29] , $H_{50\%} \geq 200$ cm (B.M., type 12 tool, 2.5 kg mass, 35 mg sample, garnet paper) ^[30] , Rotter FoI = ca. 150 ^[32] , >165 cm (US drop-hammer) ^[32] , >320 cm (NEDED) ^[43] , >320 cm (NOL) ^[43] , >320 cm (LANL) ^[43] , $H_{50} > 111.6$ ^[45] , $(H_{50}W_g)^{-1} \geq 40$ Nm ^[47] , $H_{50\%} \geq 320$ cm ^[49, 50] , $H_{50} = 490$ cm (120 J) ^[51] , 320 cm (Bruceton method, type 12 tool, 2.5 kg mass, 40 mg sample, 5/0 sandpaper, 25 trials) ^[52] , >325 cm (2.5 kg mass) ^[56] , >50 (BAM) ^[67] , 0% explosion probability @ 25 cm (10 kg mass, 50 mg powder, WL-1 type apparatus) ^[69] , $H_{50} = 150$ –170 cm (FOI = 204–224, PG-TATB, Bruceton method) ^[73] , $H_{50} = 89$ –138 cm (FOI = 109–169, UF-TATB, Bruceton method) ^[73] , $H_{50} = 490$ cm (2.5 kg mass, type 12 tool) ^[74] , $\log(H_{50}) = 2.505$ (Kamlet/Adolph) ^[75] , 114.33 (E_{dr} , Bruceton method) ^[82] , $A_{d1} = 0\%$, $A_{d2} = 0\%$, $LL = 2.0$ m, $A_{50 d1} = 10$ m, $A_{50 d2} = 8.0$ ^[98] , $H_{50\%} = 490$ cm (2.5 kg mass) ^[105]

UF-TATB, H_{50} = height of explosion with 2 kg dropweight; * = KOH was used during synthesis; # = relative humidity = 45%, $T = 306\text{ K}$ ^[73]:

Sample	Impact test [#]	
	H_{50} (cm)	Figure of insensitivity (FOI)
1*	138	169
2*	100	122
3	103	126
4	102	150
5	89	109
PG-TATB	150–170	204–224
CE (Tetryl, standard)	57	–

Rotter impact data: TATB type A, 27 mg sample, Bruceton method/25 drop run to obtain $H_{50\%}$; initiation criteria = 1 mL gas evolved or 0.5 mL accompanied by smoke or evidence of burning in the sample, data from^[103]:

Rotter impact data		US data	
F of I	Gas evolved (ml)	NSWC/NOL, ERL type 12	NWC B.M. type 12
>200	0.5	> 320 (est. 500)	> 200

FS [N]

360, 353^[6], $P_{fr,LL} = 800\text{ MPa}$ ^[21, 98], $P_{fr,50\%} = 1,300\text{ MPa}$ ^[21, 98], $F_{50} > 36\text{ kgf}$ ^[24], $F_{50} \geq 36\text{ kgf}$ ^[45], >355 (BAM)^[67], 0% explosion probability (WM-1 type apparatus)^[69], >36 kg (PG-TATB, Julius-Peter apparatus)^[73], >36 kg (UF-TATB, Julius-Peter apparatus)^[73]

UF-TATB, * = KOH was used during synthesis^[73]:

Sample	Insensitive to friction (kg)
1*	36
2*	36
3	36
4	36
5	36
PG-TATB	36
CE (Tetryl, standard)	–

ESD [J]	17.75 ^[5, 7, 9] , 293.3 mJ ^[7] , $E_{50} = 11.886$ (@ 293 K) ^[24] , $E_{50} = 13.518$ (@ 333 K) ^[24] , $E_{50} = 11.886$ ($T_0 = 293$ K) ^[45] , $E_{50} = 13.518$ ($T_0 = 333$ K) ^[45] , $E_{50\%} = 2.56 \pm 0.07$ (Bruceton method) ^[46] , $E_{50\%} = 4.25$ (LANL using 0.008 cm Pb foil confinement) ^[46] , $V_{50} = 34.12$ kV (JGY-50 type apparatus) ^[69] , $E_{50} = 17.75$ (JGY-50 type apparatus) ^[69] Data from ^[102] : <table><tr><th rowspan="2">Material</th><th colspan="3">50% point energy (J)</th></tr><tr><th>3-mil foil</th><th>10-mil foil</th><th>% expl.</th></tr><tr><td>TATB (X-398)</td><td>4.25</td><td>18.14</td><td>0</td></tr></table>			Material	50% point energy (J)			3-mil foil	10-mil foil	% expl.	TATB (X-398)	4.25	18.14	0
Material	50% point energy (J)													
	3-mil foil	10-mil foil	% expl.											
TATB (X-398)	4.25	18.14	0											
N [%]	32.56													
Ω(CO ₂) [%]	−55.78													
T _{m.p.} [°C]	>365 ^[1] , 480 ^[13] , 452 ^[13] , 330 ^[14] , 360 ^[14] , 448–449 (hot bar melting apparatus) ^[20] , >370 ^[33] , >360 ^[33, 54] , ~ 450 (dec.) ^[33] , 449 ^[34] , 374.5 (mpt. with dec., DSC, sample in sealed cell) ^[45] , 450 (dec.) ^[49, 50, 54] , >370 (Thomas Hoover Capillary Melting Point Apparatus @ 2 °C/min) ^[54] , 320 ^[58] , did not melt <593 K (PG-TATB) ^[73] , did not melt <593 K (UF-TATB) ^[73] , 544–549 K ^[101]													
T _{b.p.} [°C]	711.6 K (est., T _{nbp} , Stein-Brown method) ^[101]													
T _{dec.} [°C]	384, 330 (DTA @ 10 °C/min) ^[22] , rapid dec. >320 ^[19, 22] , 330, 350 (exotherms, DSC @ 10 °C/min) ^[19] , 450–451 (instantaneous, hot-bar) ^[19, 22] , ~ 450 ^[33] , 397 (exo peak max., DSC @ 20 °C/min) ^[34] , 375 (onset, TATB from trichlorobenzene, DSC @ 10 K/min) ^[22] , 353 (onset, TATB from trinitrobenzene/TMHI by VNS, DSC @ 10 K/min) ^[22] , 374.5 (dec., DSC, sample in sealed cell) ^[45] , 510 (5 s dec. T, 100 mg sample) ^[49] , ~ 450 (dec. of one crystal @ 2–3 °C/min heating rate from sudden exposure ~ 440 °C) ^[49] , 375.5 (onset, DSC @ 10 K/min, TATB from trichlorobenzene, 125 μm particle size) ^[62] , 374.5 (onset, DSC @ 10 K/min, TATB from tripropoxytrinitrobenzene, 103 μm particle size) ^[62] , 388.8 (exo, onset) 391.88 (exo, peak max, DSC @ 20 °C/min, 1.5 mg sample, TATB synthesized with gas-jet expansion method) ^[64] , 370.6 (DTA exo peak) ^[66] , 384.7 (exo peak max, DSC) ^[76] , 356 (DTA, exotherm onset) ^[82] , ~ 360 (no dec.) ^[85] , 235 (exo, onset), 360 (exo, peak max) (DTA) ^[100] DTA @ 6 °C/min (T _{db} = dec. begin, T _{idb} = intensive dec. beginning): T _{db} = 290 °C, T _{idb} = 350 °C ^[68] , DTA @ 6 °C/min, sample recryst. from sulfuric acid: T _{db} = ~ 180–210 °C, T _{idb} = ~ 330–350 °C ^[68]													

TATB after recryst. from DMSO, monocrystals, DTA/TGA @ 6 °C/min^[68]:

Mass of raw TATB (g)	Vol. of DMSO (mL)	Max. T of soln. (°C)	T_{db} (°C) (TGA)	T_{idb} (°C) (DTA)
1	300	145	290	350–355
0.44	150	135	2% under 260–270	360
0.32	150	130	290	360
0.2	150	110	2% under 260–270	360

Influence of crystallization, TGA @ 6 °C/min^[68]:

Sample	Average size of crystals (μm)	T_{db} (°C), (TGA @ 6 °C/min)	T_{idb} (°C) (TGA @ 6 °C/min)	ρ (g cm^{-3})
Raw TATB	8	290	350	1.927
After recryst. from aq. H_2SO_4	3–30	180–210	330–340	–
After recryst. from DMSO	25–300	230–290	350–360	1.937
TATB (monocrystals)				1.938

652 \pm 10 K (exo, DSC, @ 10 K/min, N_2 purge, 1–2 mg sample, PG-TATB)^[73], 658 K (exo, DSC, @ 10 K/min, N_2 purge, 1–2 mg sample, UF-TATB)^[73], 653 \pm 4 K (exo, 80–90% mass loss, onset = 528 \pm 10 K, DTA, @ 20 K/min, N_2 atmosphere, 1 mg sample, UF-TATB)^[73], 644 K (exo, 97% mass loss, DTA, @ 20 K/min, N_2 atmosphere, 1 mg sample, PG-TATB)^[73]

Characterization of UF-TATB by STA (DTA/TGA @ 20 K/min, N_2 atmosphere, 1 mg sample)^[73]:

Sample	DTA-exotherm peak (K)	Initial T of dec. (K)	Wt. loss on dec. (%)
1	656	525	89.67
2	651	537	80.97
3	657	523	90.02
PG-TATB	643	524	97.64

Heating rate of 8 °C/min: T_{idb} = 342.5^[26], T_w = 354.9^[26], T_{max} = 356.0^[26]
 Heating rate of 16 °C/min: T_{idb} = 351.9^[26], T_w = 366.3^[26], T_{max} = 368.2^[26],
 T_{cr} = 331–332^[26]

ρ [g cm ⁻³]	<p>1.93 (@ 293 K)^[2], 1.937^[13], 1.98^[16], 1.938 (crystal)^[25], 1.93 (crystal observed)^[14, 22, 76], 1.937 (calcd. from X-ray data)^[22], 1.938 (crystal)^[50], 1.94 (@ TMD)^[45], 1.938 (TMD)^[49, 87], 1.802 (exptl. ρ, 95% TMD)^[49, 50], 1.80 (@ 50,000 lb/in²)^[19], 1.89 (pressed TATB, 97.6% TMD, loading pressure = 64,000 psi)^[19, 49], 1.84^[58], 1.937 (@ 298 K)^[67], 1.927 (raw TATB)^[68], 1.937 \pm 0.005 (after recryst. from DMSO, pycnometry)^[68], 1.938 (monocrystals)^[68], 1.80 @ 50,000 psi^[14], 1.937 (@ TMD)^[19], 1.88 (nominal)^[19], 1.94^[99], 1.938^[99], 1.937 (crystal ρ, X-ray determined, @ 23 °C)^[20], 1.93 \pm 0.01 (direct measurement, crystal, @ 23 °C)^[20], 1.860 (pressed TATB powder @ 120 °C @ 30,000 psi)^[20]</p> <p>Data from^[85]: 1.915 (pressed, 22 °C)^[85], 1.915 \pm 0.006 (flotation with Ba(ClO₄)₂)^[85], 1.925 (99.4% TMD, He gas pycnometry)^[85], 1.935 (He gas pycnometry)^[85], 1.937 \pm 0.004 (X-ray crystallography)^[85]</p>		
Heat of formation	<p>-33.4 kcal mol⁻¹ (ΔH_f°)^[20, 85], -74.7 kJ/mol ($\Delta_f H^\circ$ (s))^[15], -541.4 kJ/kg (ICT thermochemical database)^[3], -541.3 kJ/kg (enthalpy of form.)^[18], -139.5 kJ/mol (ΔH_f)^[41], -142.7 kcal/kg (ΔH_f)^[45], -154.0 kcal/kg (enthalpy of form.)^[53], -36.85 kcal/mol^[49, 50], -0.7 kcal/mol (enthalpy of form., calcd., @ 298.15 K)^[76], -33.4--36.85 kcal/mol^[19], -154 kJ/mol ($\Delta_f H$)^[67], -154.2 kJ/mol^[87], -154.2 kJ/mol (ΔH_f)^[99]</p>		
Heat of combustion	ΔH_c° = -735.9 kcal/mol ^[25] , -735.9 kcal/mol ^[19] , ΔH_c° = -735.9 kcal/mol ^[20]		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^\circ$ [kJ kg ⁻¹]	3,866	<p>4,807 (calcd., K-J)^[15]</p> <p>2,280 (calcd., K-W)^[15]</p> <p>829 cal/g (@ 1.802 g cm⁻³)^[49, 50]</p> <p>857 cal/g (@ 1.6 g cm⁻³, calcd. Halford-Kistiakowsky equation of state)^[50]</p> <p>3,062 (calcd., ICT-code)^[3]</p> <p>922 kcal/kg (@ 1.854 g cm⁻³, calcd.) [H₂O vapor]^[53]</p> <p>1,136.4 kJ/mol ($\Delta_{\text{ex}}H$)^[67]</p> <p>4.402 kJ g⁻¹ ($\Delta_{\text{ex}}H$)^[67]</p>	<p>3,062 [H₂O (l)]^[12, 18, 76]</p> <p>2,831 cal/g^[14, 19]</p> <p>1,018 cal/g (@ 1.87 g cm⁻³) [H₂O (g)]^[19]</p> <p>2,831 cal/g (@ 1.87 g cm⁻³) [H₂O (l)]^[19]</p> <p>949 kcal/kg (@ 1.854 g cm⁻³) [H₂O vapor]^[53]</p> <p>920 kcal/kg (@ 1.84 g cm⁻³, Q_{exp})^[71]</p> <p>829 cal/g (@ 1.80 g cm⁻³, based on watershed measurements)^[76]</p>

		<p>3,992 MJ•kg⁻¹ (Q_{real}, calcd., semi-empirical Pepekin method)^[82]</p> <p>1,018 ± 10 cal/g (heat of detonation)^[85]</p> <p>1,076 cal/g (heat of detonation)^[85]</p> <p>$-\Delta H_{\text{det}} = 4.49 \text{ kJ/g}$^[99]</p> <p>Heat of det. = -5.02 MJ/kg^[99]</p>	808 cal/g (@ 1.50 g cm ⁻³ , based on watershock measurements) ^[76]
T_{ex} [K]	2,760	<p>2,574 (@ 1.6 g cm⁻³, calcd. Halford–Kistiakowsky equation of state)^[50]</p> <p>2,218 (calcd., ICT-code)^[3]</p> <p>1,887 (@ 1.895 g cm⁻³, calcd., <i>Mader</i>, BKW)^[76]</p> <p>1,890 (@ 1.895 g cm⁻³, calcd., <i>Borg</i>, SDA FOR code)^[76]</p> <p>2,393 (@ 1.937 g cm⁻³, $\Delta H_f = -140 \text{ kJ/mol}$, calcd., JAGUAR)^[97]</p> <p>2,550 (@ 1.88 g cm⁻³, calcd. BKWR)^[17]</p> <p>2,580 (@ 1.85 g cm⁻³, calcd. BKWR)^[17]</p> <p>3,250 (@ 1.88 g cm⁻³, calcd. BKWS)^[17]</p> <p>3,260 (@ 1.85 g cm⁻³, calcd. BKWR)^[17]</p>	
$p_{\text{C-I}}$ [kbar]	283	<p>287 (calcd., K-J)^[15]</p> <p>282 (calcd., K-W)^[15]</p> <p>270 (@ 1.847 g cm⁻³, calcd., CHEETAH 2.0)^[8]</p> <p>283 (calcd., K-J)^[25]</p>	<p>259 (@ 1.847 g cm⁻³)^[8]</p> <p>326 (@ 1.895 g cm⁻³)^[13]</p> <p>255.6 (@ 1.847 g cm⁻³)^[13]</p> <p>172 (@ 1.5 g cm⁻³)^[13]</p>

		<p>259 (@ 1.802 g cm⁻³)^[49, 50]</p> <p>171.2 (@ 1.6 g cm⁻³, calcd. Halford–Kistiakowsky equation of state)^[50]</p> <p>96.1 MPa (calcd., ICT-code)^[3]</p> <p>0.326 MPa (@ 1.895 g cm⁻³, calcd., <i>Mader</i>, BKW)^[76]</p> <p>0.325 MPa (@ 1.895 g cm⁻³, calcd., <i>Borg</i>, SDA FOR code)^[76]</p> <p>31.8 GPa (@ 1.937 g cm⁻³, $\Delta H_f = -140$ kJ/mol, calcd., JAGUAR)^[97]</p> <p>328 (@ 1.88 g cm⁻³, calcd. BKWR)^[17]</p> <p>314 (@ 1.85 g cm⁻³, calcd. BKWR)^[17]</p> <p>285 (@ 1.88 g cm⁻³, calcd. BKWS)^[17]</p> <p>271 (@ 1.85 g cm⁻³, calcd. BKWR)^[17]</p>	<p>259 (@ 1.85 g cm⁻³)^[17]</p> <p>315^[15]</p> <p>313 (@ crystal ρ)^[19]</p> <p>25.2 GPa (@ 1.83 g cm⁻³)^[38]</p> <p>25.9 GPa (@ 1.847 g cm⁻³)^[20]</p> <p>17.5 GPa (@ 1.50 g cm⁻³)^[20]</p> <p>259.4 (@ 1.80 g cm⁻³, based on watershed measurements)^[76]</p> <p>174.6 (@ 1.50 g cm⁻³, based on watershed measurements)^[76]</p>
VoD [m s ⁻¹]	8,327	<p>7,930 (@ 1.895 g cm⁻³, calcd., K-J)^[15]</p> <p>7,850 (@ 1.895 g cm⁻³, calcd., K-W)^[15]</p> <p>7,814 (@ 1.847 g cm⁻³, calcd., CHEETAH 2.0)^[8]</p> <p>8,000 (@ 1.94 g cm⁻³, calcd., K-J)^[29]</p> <p>7,950 (@ 1.938 g cm⁻³, calcd., K-J)^[25]</p> <p>7,980 (@ 1.94 g cm⁻³ (TMD), calcd., K-J)^[36]</p> <p>8,340 (@ 1.94 g cm⁻³ (TMD), calcd., <i>Aizenshtadt</i>)^[36]</p>	<p>8,000 (@ 1.937 g cm⁻³)^[19]</p> <p>7.99 km/s (@ 1.938 g cm⁻³)^[25]</p> <p>7,660 (@ 1.847 g cm⁻³)^[8]</p> <p>7,760 (@ 1.88 g cm⁻³)^[10, 12, 17]</p> <p>7,660 (@ 1.85 g cm⁻³)^[10, 12, 17]</p> <p>7,940 (@ 1.95 g cm⁻³)^[11]</p> <p>7,666 (@ 1.847 g cm⁻³)^[13]</p> <p>8,411 (@ 1.895 g cm⁻³)^[13]</p> <p>7,500 (@ 1.80 g cm⁻³, 0.5 in charge diameter, pressed, no confinement)^[14]</p>

		<p>7,870 (@ 1.94 g cm⁻³ (TMD), calcd., R-P method)^[36]</p> <p>7,539 (@ 1.86 g cm⁻³)^[37, 44]</p> <p>7,658 (@ 1.802 g cm⁻³)^[49, 50]</p> <p>7,055 (@ 1.6 g cm⁻³, calcd. Halford–Kistiakowsky equation of state)^[50]</p> <p>8,411 (@ 1.895 g cm⁻³, calcd., <i>Mader</i>, BKW)^[76]</p> <p>8,365 (@ 1.895 g cm⁻³, calcd., <i>Borg</i>, SDA FOR code)^[76]</p> <p>7,920 (@ TMD, calcd., K-J)^[82]</p> <p>8,310 (@ 1.937 g cm⁻³, $\Delta H_f = -140$ kJ/mol, calcd., JAGUAR)^[97]</p> <p>8,280 (@ 1.88 g cm⁻³, calcd. BKWR)^[17]</p> <p>8,180 (@ 1.85 g cm⁻³, calcd. BKWR)^[17]</p> <p>8,190 (@ 1.88 g cm⁻³, calcd. BKWS)^[17]</p> <p>8,070 (@ 1.85 g cm⁻³, calcd. BKWR)^[17]</p>	<p>5,380 (@ 1.290 g cm⁻³)^[14]</p> <p>5,628 (@ 1.345 g cm⁻³)^[14]</p> <p>6,550 (@ 1.675 g cm⁻³)^[14]</p> <p>6,575 (@ 1.675 g cm⁻³)^[14]</p> <p>7,035 (@ 1.882 g cm⁻³)^[14]</p> <p>7,220 (@ 1.835 g cm⁻³)^[14]</p> <p>7,619 ± 0.001 (@ 1.860 g cm⁻³, Cu tube, 25.35 mm charge diameter, confined)^[20]</p> <p>7,660 (@ 1.847 g cm⁻³)^[20]</p> <p>7,510 (@ 1.84 g cm⁻³)^[22]</p> <p>7,570 (@ 1.80 g cm⁻³)^[38]</p> <p>7,660 (@ 1.85 g cm⁻³)^[38]</p> <p>7,860 (@ 1.90 g cm⁻³)^[38]</p> <p>7,640 (@ 1.83 g cm⁻³)^[38]</p> <p>7,658 (@ 1.80 g cm⁻³, based on watershock measurements)^[76]</p> <p>6,555 (@ 1.50 g cm⁻³, based on watershock measurements)^[76]</p> <p>7,350 (@ 1.80 g cm⁻³)^[82]</p> <p><i>See additional values at end of section</i></p>
V_0 [L kg ⁻¹]	676	0.4906 cm ³ /g (@ 1.6 g cm ⁻³ , calcd. Halford–Kistiakowsky equation of state) ^[50]	

Detonation velocities of TATB, values from^[50]:

Charge no.	Diameter (cm)	Length (cm)	Confinement	ρ (g cm ⁻³)	VoD (m/s)
1 (boosted by 75/25 cyclotol) [†]	Conical	0.64	None	1.880	-
	0.64	1.27	None	1.881	-
	1.27	1.32	None	1.874	7,610
	1.27	1.35	None	1.879	7,610
	1.27	1.35	None	1.880	7,610
	1.27	1.32	None	1.878	7,614
	2.54	2.57	None	1.882	7,772
	2.54	2.57	None	1.875	7,772
2 (boosted by Tetryl) [‡]	Conical		None	1.864	7,650
	1.27	2.54	None	1.863	7,650
	2.54	2.54	None	1.860	7,745
	2.54	2.54	None	1.864	7,745
	5.08	5.08	None	1.862	7,745
	5.08	5.08	None	1.864	7,745
3	5.08	5.08	Glass	1.802	7,658
4	4.45	15.24	Glass	1.508	6,555

[†] tapered to 0.31 cm from 0.64 cm over 0.64 cm length. Detonation did not propagate into 0.64 cm diameter section^[50]

[‡] tapered to 0.64 diameter from 1.27 cm diameter over 1.9 cm length^[50]

Chapman–Jouguet pressure, energy and isentropic exponent from H₂O-shock measurements^[19, 50]:

ρ (g cm ⁻³)	VoD (m/s)	U_{H_2O} (m/s)	u_{H_2O} (m/s)	P_{H_2O} @ HE•H ₂ O interface (kb)	p_{C-J} (kb)	k	Q (cal/g)
1.80	7,658	6,071	2,685	163.0	259.4	3.07	829
1.50	6,555	5,519	2,303	126.9	174.6	2.71	808

Summary of experimental copper cylinder wall velocity data, PETN with a density of 1.763 g/cm³ is the reference explosive, data from^[87]:

Initial density (g/cm ³)	Inner diameter (mm)	Wall thickness (mm)	Wall velocity (mm/μs) at 25.4 mm diameter for R-R ₀ equal to			Velocity-squared cf. with PETN for the same configuration, % comparison R-R ₀ equal to		
			6 mm	12.5 mm	19 mm	6 mm	12.5 mm	19 mm
1.83	50.81	5.207	1.300	1.403	1.453	-30.6	-32.3	-34.1

Summary of code calculations with measure detonation velocities and detonation energies derived from JWL's^[87]:

Initial density (g/cm ³)	PETN-adjusted BKWR Tiger, LLNL library, $\theta = 1,850$ K, at v			JCZ3, LLNL library, v			CHEQ V2.4, at v		
	2.2 mm	4.1 mm	6.5 mm	2.2 mm	4.1 mm	6.5 mm	2.2 mm	4.1 mm	6.5 mm
1.83	3	1	3	6	4	4	8	7	9

Derivation of the total energy of detonation, E_0 from the measured heat of detonation. The final state is assumed to be at one atmosphere for all gaseous products including water at 298 K. Code calculated energies with the 1,800 K freeze are also included, data from^[87]:

Measured density (g/cm ³)	Measured confined heat of detonation (kJ/cm ³)	Density from ^[87]	Heat of detonation using density from ^[87]	Energy of detonation, E_0 (kJ/cm ³)			
				From heat of detonation	Freeze at 1,800 K		
					Tiger BKWR	Tiger JCZ3	CHEQ
1.87	-7.96	1.86	-7.92	-7.5	-6.8	-7.0	-7.7

JWL cylinder coefficients data from^[87]:

Initial density, ρ_0 (g/cm ³)	Detonation velocity, D (mm/μs)	Energy of detonation, E_0 (kJ/cm ³)	CJ pressure (GPa)	A (GPa)	B (GPa)	C (GPa)	R_1	R_2	ω	γ_{CJ}
1.83	7.58	-7.30	26.0	686.8140	7.811448	0.877917	4.958	1.20	0.30	3.044

Critical diameter [cm]	<p>Critical diameter = 7.94 ± 1.6 mm; $\rho = 1.71$ g cm⁻³^[35], critical diameter = 13 mm; $\rho = 1.80$–1.84 g cm⁻³^[35], critical diameter = 4 mm; $\rho = 1.86$–1.88 g cm⁻³^[35]</p> <p>Critical diameters for pressed TATB^[48]: 6.35 mm < d_c < 9.53 mm (60 μm particle size, $\rho = 1.6$–1.7 g cm⁻³, (82.6–87.7% TMD))^[48], < 6.35 mm (20 μm particle size, $\rho = 1.6$–1.7 g cm⁻³ (82.6–87.7% TMD))^[48], $d_c = 13$ mm (@ 1.802 g cm⁻³, 92.7% TMD, pressed TATB)^[55]</p> <p>$d_c = 13$ mm @ 93% TMD TATB, fine)^[83]</p> <p>Failure diameter = 4.0 mm (TATB pressed to $\rho = 1.860$ g cm⁻³)^[20]</p> <p>Data from^[94]:</p> <table><tr><th rowspan="2">ρ_0 (g/cc)</th><th rowspan="2">% TMD</th><th rowspan="2">d_c (cm)</th><th rowspan="2">Gap test no.</th><th colspan="4">50% point</th></tr><tr><th>ρ_0 (g/cc)</th><th>% TMD</th><th>no. cards</th><th>P_g (kbar)</th></tr><tr><td>1.802</td><td>92.7</td><td>1.3</td><td>499</td><td>1.82</td><td>94.6</td><td>78</td><td>64</td></tr></table>	ρ_0 (g/cc)	% TMD	d_c (cm)	Gap test no.	50% point				ρ_0 (g/cc)	% TMD	no. cards	P_g (kbar)	1.802	92.7	1.3	499	1.82	94.6	78	64																																								
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Critical T [°C]	<p>331–332 (exptl.)^[57, 78], 334 (calcd.)^[57, 78], 913 K^[76], 912.7 K (est., Joback-Stein method)^[101], 1,189.0 K (Valderrama–Alveraz method)^[101], 347 (T_m)^[20]</p> <p>Critical T of TATB measured by various methods, values from^[85]:</p> <table><tr><th>Type of TATB</th><th>Pressed thickness (mm)</th><th>T_c (°C)</th><th>Test</th></tr><tr><td>Recryst. from DPE</td><td>0.65</td><td>354</td><td>Henkin (LANL)</td></tr><tr><td>Cordova</td><td>0.67</td><td>355</td><td>Henkin (LANL)</td></tr><tr><td>Hercules</td><td>0.63</td><td>358</td><td>Henkin (LANL)</td></tr><tr><td>Recryst. from DMSO</td><td>0.68</td><td>345</td><td>Henkin (LANL)</td></tr><tr><td>Rocketdyne</td><td>0.55</td><td>357</td><td>Henkin (LANL)</td></tr><tr><td>Recryst. from H₂SO₄</td><td>0.61</td><td>354</td><td>Henkin (LANL)</td></tr><tr><td>TATB</td><td></td><td>352</td><td>Henkin (LANL)</td></tr><tr><td>TATB-d₆</td><td>0.61</td><td>366</td><td>Henkin (LANL)</td></tr><tr><td>TATB</td><td></td><td>312</td><td>Gilding metal</td></tr><tr><td>TATB</td><td>0.66</td><td>331–332</td><td>Al cell</td></tr><tr><td>Recryst. from dmso</td><td>~ 0.8</td><td>345–355</td><td>Al cell</td></tr><tr><td>Cordova</td><td>~ 0.8</td><td>345–355</td><td>Al cell</td></tr><tr><td>TATB</td><td></td><td>256</td><td>ODTX, $\rho = 0.284$ cm</td></tr><tr><td>TATB</td><td></td><td>230</td><td>ODTX, $\rho = 0.635$ cm</td></tr></table>	Type of TATB	Pressed thickness (mm)	T_c (°C)	Test	Recryst. from DPE	0.65	354	Henkin (LANL)	Cordova	0.67	355	Henkin (LANL)	Hercules	0.63	358	Henkin (LANL)	Recryst. from DMSO	0.68	345	Henkin (LANL)	Rocketdyne	0.55	357	Henkin (LANL)	Recryst. from H ₂ SO ₄	0.61	354	Henkin (LANL)	TATB		352	Henkin (LANL)	TATB-d ₆	0.61	366	Henkin (LANL)	TATB		312	Gilding metal	TATB	0.66	331–332	Al cell	Recryst. from dmso	~ 0.8	345–355	Al cell	Cordova	~ 0.8	345–355	Al cell	TATB		256	ODTX, $\rho = 0.284$ cm	TATB		230	ODTX, $\rho = 0.635$ cm
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Critical pressure [bar]	56.5 ^[76] , 56.45 (est., Joback-Stein method) ^[101] , 31.14 (Valderrama-Alveraz method) ^[101]																																
Critical pressure of explosion initiation [GPa]	$P_{cr} = 1.25 \pm 0.04$ ^[63] , $P_{cr} = 1.11$ ^[71] , $\sigma_{ult} = 102$ MPa ^[71]																																
Trauzl test [cm ³ , % TNT]	175 ^[96]																																
Sand test [g]	42.9 g (200 g bomb) ^[14, 19] , 90% TNT ^[19]																																
Initiation efficiency	0.30 g LA minimum detonating charge ^[14, 19]																																
Plate dent test [mm]	<p>5.87 crater depth (@ 1.86 g cm⁻³)^[44], plate dent = 4.42 mm @ 1.753 g cm⁻³, 41.3 mm diameter samples, est. $p_{C-I} = 245$ kbar^[85]</p> <p>Data from^[20]:</p> <table><tr><td>Charge diameter (mm)</td><td>Density (g/cm³)</td><td>Dent depth (mm)</td><td>Charge height (mm)</td></tr><tr><td>41.3</td><td>1.87</td><td>8.31</td><td>203</td></tr></table>			Charge diameter (mm)	Density (g/cm ³)	Dent depth (mm)	Charge height (mm)	41.3	1.87	8.31	203																						
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41.3	1.87	8.31	203																														
Gap test	<p>Gap test >50 kbar, charge $\rho = 1.84$ g cm⁻³^[23], gap test >50 kbar, charge $\rho = 1.63$ g cm⁻³ (cast TATB)^[23], gap test >50 kbar, charge $\rho = 1.86$ g cm⁻³^[44], $G_{50} = 27.92$ mm (@ 1.87 g cm⁻³, 96.4% TMD)^[65]</p> <p>Los Alamos standard gap test (pressures from calibration curve, sample $\rho = 1.870$ g cm⁻³, calculation based on limited plot data for sample with $\rho = 1.876$ g cm⁻³)^[77]:</p> <table><tr><td>Gap (mm)</td><td>14.4</td><td>20.6</td></tr><tr><td>Pressures (GPa):</td><td>23.2</td><td>19.0</td></tr><tr><td>Dural gap</td><td colspan="2"></td></tr><tr><td>Induced in sample</td><td colspan="2"></td></tr><tr><td>Calculation</td><td>23.5</td><td>13.5</td></tr><tr><td>Independence match</td><td>16.3</td><td>13.0</td></tr><tr><td>Run distance (mm)</td><td colspan="2"></td></tr><tr><td>Pop plot</td><td>3</td><td>6</td></tr><tr><td>Calculation</td><td>7</td><td>-</td></tr><tr><td>Exptl. 50% gap (mm)</td><td colspan="2">21.9</td></tr></table>			Gap (mm)	14.4	20.6	Pressures (GPa):	23.2	19.0	Dural gap			Induced in sample			Calculation	23.5	13.5	Independence match	16.3	13.0	Run distance (mm)			Pop plot	3	6	Calculation	7	-	Exptl. 50% gap (mm)	21.9	
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SSGT results for TATB^[19]:

	Density (g/cm ³)	% voids	Sensitivity (mm)
PX gap test	1.883 (pressed)	-	Approx. 5.3
	1.861 (pressed)	4.0	5.61
	1.700 (pressed)	12.3	14.10
	1.03 (bulk)	-	102–16.3

L = LSGT (41.275 mm), M = PGXT (24.5 mm), S = SSGT (12.7 mm), ** μ = particle size, ** blm = ball milled, data from^[85].

Density (g/cm ³)	Voids (%)	50% point (mm)	Test	Ref.	Comments
1.7		0–0.025	S	LANL	50 μ **
1.7		0.042	S	LANL	20 μ
1.7		0.025–0.051	S	LANL	5 μ
1.881	2.9	22.78	L	LANL	
1.883		5.17	M	LANL	
1.865	3.8	0.127	S	LANL	Prod
1.750	9.7	0.36	S	LANL	1.5% Cl superfine
1.700		0.38	S	LANL	13 μ
1.700		0.36	S	LANL	0.2% Cl
1.700		0.38	S	LANL ~ 20 μ , 0.15% Cl	
1.700		0.05	S	LANL	Fine
1.600	17.4	0.36	S	LANL	1.5% Cl superfine
1.200	38.1	0.20	S	LANL	1.5% Cl superfine
1.000	48.4	0.13	S	LANL	Superfine
0.777	60.0	0.13	S	LANL	Superfine

NOL LSGT

20 mm (78 cards) (50% probability point)^[42], $P_{50} = 6.58$ GPa (@ 1.82 g cm⁻³)^[67]

LANL LSGT ²	<div>LANL LSGT data from^[19]:</div> <table><tr><td>Density (g/cm³)</td><td>% Voids</td><td>Sensitivity (mm)</td></tr><tr><td>1.786 (pressed)</td><td>2.8</td><td>41.68</td></tr><tr><td>1.705 (pressed)</td><td>7.2</td><td>45.36</td></tr><tr><td>0.81 (bulk)</td><td>56</td><td>49.3</td></tr></table> <div>21.92 mm (@ 1.86–1.88 g cm⁻³)^[35]</div>	Density (g/cm ³)	% Voids	Sensitivity (mm)	1.786 (pressed)	2.8	41.68	1.705 (pressed)	7.2	45.36	0.81 (bulk)	56	49.3																													
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LSGT [cm]	<div>$G_{50} = 21.92$ mm, $L_{95} = 0.43$ mm @ 1.870 g cm⁻³^[20], 10 mm (NOL)^[43], 18 mm (LANL)^[43], $L_g = 78$ in $\times 10^2$ (@ 1.82 g cm⁻³, 94.6% TMD, pressed TATB, NSW LSGT)^[55]</div> <div>Comparison of NOL LSGT results with those of IHE gap test^[39]:</div> <table><tr><td>Material</td><td>ρ_0 (g cm⁻³)</td><td>IHE (50% gap, in)</td><td>LSGT (in $\times 10^2$)</td></tr><tr><td>TATB</td><td>1.83</td><td>0.92</td><td>78–84</td></tr></table> <div>Conversion of SSGT values to LSGT values, TATB X335^[83]:</div> <table><tr><th rowspan="2">ρ_0 (g/cc)</th><th rowspan="2">% TMD</th><th colspan="3">50% point</th></tr><tr><th>DBG</th><th>SSGT, P_g (kbar)</th><th>LSGT, P_g (kbar)</th></tr><tr><td>1.519</td><td>78.38</td><td>7.92</td><td>43.2</td><td>33.7</td></tr><tr><td>1.645</td><td>84.88</td><td>8.56</td><td>52.5</td><td>39.3</td></tr><tr><td>1.762</td><td>90.92</td><td>9.63</td><td>74.1</td><td>48.8</td></tr><tr><td>1.840</td><td>94.94</td><td>11.10</td><td>117.5</td><td>62.5</td></tr><tr><td>1.887</td><td>97.37</td><td>13.47</td><td>162.2</td><td>83.0</td></tr></table> <div>Pressed TATB @ 1.70 g cm⁻³ (90% TMD), gap material = Ly-12A1, $G_{50} = 28.0$ mm^[88], TMD = 1.938 g cm⁻³, exptl. $\rho = 1.83$ g cm⁻³, 94.2% TMD, gap = 78 cards^[93], $\rho_0 = 1.82$ g/cc, 93.9% TMD, 50% pressure (P_g) = 64.0 kbar^[94]</div>	Material	ρ_0 (g cm ⁻³)	IHE (50% gap, in)	LSGT (in $\times 10^2$)	TATB	1.83	0.92	78–84	ρ_0 (g/cc)	% TMD	50% point			DBG	SSGT, P_g (kbar)	LSGT, P_g (kbar)	1.519	78.38	7.92	43.2	33.7	1.645	84.88	8.56	52.5	39.3	1.762	90.92	9.63	74.1	48.8	1.840	94.94	11.10	117.5	62.5	1.887	97.37	13.47	162.2	83.0
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SSGT [cm]	<div>Data from^[19]:</div> <table><tr><td></td><td>Density (g/cm³)</td><td>% Voids</td><td>Sensitivity (mm)</td></tr><tr><td rowspan="2">NSWC SSGT</td><td>1.887</td><td>2.2</td><td>1.12</td></tr><tr><td>1.519</td><td>21.3</td><td>4.12</td></tr><tr><td>LANL SSGT</td><td>1.872</td><td>3.4</td><td>0.13</td></tr></table>		Density (g/cm ³)	% Voids	Sensitivity (mm)	NSWC SSGT	1.887	2.2	1.12	1.519	21.3	4.12	LANL SSGT	1.872	3.4	0.13																										
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$G_{50} = 0.127$ mm, $L_{95} = 0.10$ mm @ 1.872 g cm⁻³[20], 1.0 mm (NOL)^[43],
 $P_{90} = 46.20$ kbar (P_{90} = pressure to 90% of TMD, NSW small-scale gap test)^[52]

Conversion of SSGT values to LSGT values, TATB X335^[83]:

ρ_0 (g/cc)	% TMD	50% point		
		DBG	SSGT, P_g (kbar)	LSGT, P_g (kbar)
1.519	78.38	7.92	43.2	33.7
1.645	84.88	8.56	52.5	39.3
1.762	90.92	9.63	74.1	48.8
1.840	94.94	11.10	117.5	62.5
1.887	97.37	13.47	162.2	83.0

TATB TMD = 1.93, all samples loaded under vacuum^[92]:

Loading pressure (kpsi)	Density (g/cm ³)		% TMD	Sensitivity (DBG)			
	AVG.	s		AVG.	g	s_m	N
4	1.519	0.010	78.7	7.918	0.0291	0.0316	20
8	1.645	0.008	85.2	8.573	0.0657	0.0390	20
16	1.762	0.005	91.3	9.626	0.0596	0.0358	20
32	1.840	0.003	95.3	11.091	0.0599	0.0415	20
64	1.887	0.004	97.8	13.606	0.2150	0.1277	20

TATB, TMS = 1.93 g cm⁻³, no mixed response zone^[92]:

Loading pressure (kpsi)	Density (g/cm ³)		% TMD	Sensitivity (DBG)			
	AVG.	s		AVG.	g	s_m	N
8	1.727	0.0025	89.5	9.352	—	—	20

$\rho_0 = 1.82$ g/cc, 93.9% TMD, 50% pressure (P_g) = 102 kbar (nominal value, beyond range of calibration)^[94], 16.5 GPa (@ 98% TMD, NSW)^[99]

Underwater SSGT (USGT)

L_c (critical length) = 1 mm^[24, 45]

Small-scale gap (booster) sensitivity test

Pressed TATB^[49]:

@ 93% TMD		@ 95% TMD	
DBg	Lucite gap (mils)	DBg	Lucite gap (mils)
10.1	98	11.1	78

5 s explosion T [°C] Explosion T [°C]	520 ^[19]						
	373 (DTA/TG @ 6 °C/min) ^[23]						
	Temperature (°C) and time (s) to explosion (ODTX) ^[85] :						
	Temperature (°C)		Time (s)				
	215		22,680				
	216		21,744				
	215		24,624				
	Henkin times to explosion for various lots of TATB at 368 °C, Al blasting caps and Lee plugs, 80 mg sample size ^[85] :						
	Type of TATB	Particle size		Total Cl (%)	Time to explosion (s)	Averages from number	
		% < 20 µm	% < 44 µm			Of samples	Of tests
	Pantex	13	43	0.68	149	3	4
	Cordova	19	39	0.63	133	2	4
	Teledyne	94	16	3.45	39	1	4
Ignition T [K]	No ignition <623 K (PG-TATB) ^[73] , no ignition <623 K (UF-TATB) ^[73] , 355 ^[82]						
Autoignition point [°C]	320–325 ^[19]						
Thermal stability [no. moles gas per mole TATB/no. hours]	@ 120 °C: 0/22, 0/72 ^[34] , @ 220 °C: 0/22, 0/72 ^[34] , @ 320 °C: 3.23/22, 3.40/72, 3.84/ >416 ^[34] , 2cc/g/h for 2 h period @ 280 °C ^[49] , autocatalytic dec. @ 300 °C in 95 min ^[49]						
Thermal stability	0.06% mass loss @ 120 °C, 48 h ^[66] , 245 °C (threshold of thermal stability) ^[82] , ~ 11% mass loss after 2 weeks @ 204 °C ^[85]						
Heat test	@ 100 °C: 0.00% loss in first 48 h ^[14] , 0.00% loss in second 24 h ^[14] , no explosions in 100 h ^[14] @ 200 °C: 0.5 cm ³ gas evolved in 48 h ^[19] @ 220 °C: 2.3 cm ³ gas evolved in 48 h ^[19] @ 260 °C: 1.2 cm ³ gas evolved in 1 h ^[19] @ 280 °C: 2.0 cm ³ gas evolved in 1 h ^[19]						

Vacuum stability test [cm ³ /time]	<p>0.36 cc/40 h @ 100 °C^[14], 0.0–0.2 mL/g of gas evolved after 48 h @ 120 °C^[20], 0.10 mL/5 g @ 120 °C, 48 h^[66]</p> <p>@ 150 °C: 0.2/2 days, 0.3/7 d, 0.3/14 d, 0.4/21 d, 0.4/28 d, 0.4/35 d, 0.4/42 d, 0.4/49 d, 0.5/56 d, 0.5/63 d, 0.5/70 d, 0.5/77 d, 0.6/84 d^[31]</p> <p>@ 175 °C: 0.3/2 days, 0.4/7 d, 0.4/14 d, 0.5/21 d, 0.6/28 d, 0.7/35 d, 0.8/42 d, 0.9/49 d, 1.0/56 d, 1.1/63 d, 1.2/70 d, 1.4/77 d, 1.5/84 d, 1.6/91 d^[31]</p> <p>@ 200 °C: 0.3/2 days, 0.9/7 d, 2.1/14 d, 4.1/21 d, 7.2/28 d, 11.1/35 d, 15.8/42 d^[31]</p> <p>@ 200 °C (TATB recryst. from DMSO): 1.0/2 days, 4.7/7 d, 12.5/14 d, 20.0/21 d^[31]</p> <p>@ 120 °C (TATB from tripropoxytrinitrobenzene): 0.0–0.2 cm³/40 h^[22], @ 120 °C (TATB from trichlorobenzene): 0.2 cm³/40 h^[22], @ 100 °C: 0.0 cc/g/48 h^[49], @ 260 °C: 0.7 cc/g/h (average for 2 h exposure)^[49], @ 280 °C: 2.0 cc/g/h (average for 2 h exposure)^[49], @ 100 °C: 0.1 cm³/g/48 h^[50], @ 260 °C: 0.8 cm³/g/h (average for 2 h exposure)^[50], @ 280 °C: 4.5 cm³/g/h (average for 2 h exposure)^[50], 0.2 cm³ (@ 120 °C, 40 h, TATB from trichlorobenzene, 125 µm particle size)^[62], 0.0–0.2 cm³ (@ 120 °C, 40 h, TATB from tripropoxytrinitrobenzene, 103 µm particle size)^[62], 0.206 mL/5 g @ 94 °C for 48 h^[100]</p> <p>VTS/CRT data from^[85]:</p> <table border="1"> <thead> <tr> <th>Gas evolution (cm³/g/h/°C)</th><th>Test used</th></tr> </thead> <tbody> <tr><td>0.36/48 h/100 °C</td><td>CRT</td></tr> <tr><td>6.0/2 h/260 °C</td><td>CRT ($\rho = 1.934$)</td></tr> <tr><td>11.5/0.5 h/300 °C</td><td>CRT</td></tr> <tr><td>0.0–0.5/48 h/120 °C</td><td>VTS</td></tr> <tr><td>0.2/48 h/150 °C</td><td>VTS</td></tr> <tr><td>0.3/168 h/150 °C</td><td>VTS</td></tr> <tr><td>0.3/48 h/175 °C</td><td>VTS</td></tr> <tr><td>0.36/48 h/200 °C</td><td>VTS</td></tr> <tr><td>0.9/168 h/200 °C</td><td>VTS</td></tr> <tr><td>1.0/48 h/200 °C</td><td>VTS (DMSO recryst.)</td></tr> <tr><td>4.7/168 h/200 °C</td><td>VTS (DMSO recryst.)</td></tr> <tr><td>0.5/48 h/200 °C</td><td>VTS</td></tr> <tr><td>2.3/48 h/220 °C</td><td>VTS</td></tr> <tr><td>18.9/34 h/240 °C</td><td>VTS</td></tr> <tr><td>0.0/2 h/200 °C</td><td>VTS (fine)</td></tr> <tr><td>0.2/2 h/225 °C</td><td>VTS</td></tr> <tr><td>1.1/2 h/250 °C</td><td>VTS</td></tr> <tr><td>1.8/2 h/275 °C</td><td>VTS</td></tr> <tr><td>19.8/2 h/300 °C</td><td>VTS</td></tr> <tr><td>92.8/1 h/320 °C</td><td>VTS</td></tr> </tbody> </table>	Gas evolution (cm ³ /g/h/°C)	Test used	0.36/48 h/100 °C	CRT	6.0/2 h/260 °C	CRT ($\rho = 1.934$)	11.5/0.5 h/300 °C	CRT	0.0–0.5/48 h/120 °C	VTS	0.2/48 h/150 °C	VTS	0.3/168 h/150 °C	VTS	0.3/48 h/175 °C	VTS	0.36/48 h/200 °C	VTS	0.9/168 h/200 °C	VTS	1.0/48 h/200 °C	VTS (DMSO recryst.)	4.7/168 h/200 °C	VTS (DMSO recryst.)	0.5/48 h/200 °C	VTS	2.3/48 h/220 °C	VTS	18.9/34 h/240 °C	VTS	0.0/2 h/200 °C	VTS (fine)	0.2/2 h/225 °C	VTS	1.1/2 h/250 °C	VTS	1.8/2 h/275 °C	VTS	19.8/2 h/300 °C	VTS	92.8/1 h/320 °C	VTS
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Burn rate [mm/s]	2.0 @ 100 atm. pressure ^[59] , 10.0 @ 600 atm. pressure ^[59] , 15.0 @ 1,000 atm. pressure ^[59] , TATB does not sustain self-deflagration @ pressure ≤ 10.34 MPa ^[85] , self-deflagration is an order of magnitude lower than that of HMX @ 13–103 MPa ^[85]																																																														
Solubility [g/mL]	<p>Solubility >20% by wt. per vol. of soln. in superacids such as conc. sulfuric acid, chlorosulfonic acid, fluorosulfonic acid and trifluoromethane sulfuric acid^[19]</p> <p>Solubility data from^[19]:</p> <table border="1"> <thead> <tr> <th>Solvent</th><th>Solubility (ppm)</th><th>Solvent</th><th>Solubility (ppm)</th></tr> </thead> <tbody> <tr> <td>Methanesulfonic acid</td><td>820</td><td><i>N</i>-Methylformamide</td><td>6</td></tr> <tr> <td>Hexamethylphosphortriamide</td><td>150</td><td>Methyl methanesulfonate</td><td>5</td></tr> <tr> <td>Ethanesulfonic acid</td><td>120</td><td>Trimethylphosphite</td><td>4</td></tr> <tr> <td>DMSO</td><td>70</td><td>Acetone</td><td>3</td></tr> <tr> <td>Hexafluoroacetone sesquihydrate</td><td>68</td><td>Dimethyl carbamoyl chloride</td><td>3</td></tr> <tr> <td><i>N</i>-Methyl-2-pyrrolidinone</td><td>58</td><td>Acetonitrile</td><td>3</td></tr> <tr> <td><i>N,N</i>-Dimethylacetamide</td><td>33</td><td>Acetic anhydride</td><td>3</td></tr> <tr> <td>DMF</td><td>27</td><td>Trifluoroacetic acid</td><td>3</td></tr> <tr> <td>Tetramethylurea</td><td>26</td><td>Acetic acid</td><td>1</td></tr> <tr> <td>Dimethyl methylphosphonate</td><td>22</td><td>Hexamethyldisilazane</td><td>Less than 1</td></tr> <tr> <td><i>N,N</i>-Dimethylpropionamide</td><td>16</td><td>Trifluoroacetic anhydride</td><td>Less than 1</td></tr> <tr> <td>Bis(dimethylamino) phosphochloridate</td><td>14</td><td>Hexafluorobenzene</td><td>Less than 1</td></tr> <tr> <td>Gamma butyrolactone</td><td>14</td><td>Pentafluoropyridine</td><td>Less than 1</td></tr> <tr> <td>Conc. nitric acid</td><td>14</td><td>Perfluoro-2-butyltetrahydrofuran</td><td>Less than 1</td></tr> </tbody> </table>			Solvent	Solubility (ppm)	Solvent	Solubility (ppm)	Methanesulfonic acid	820	<i>N</i> -Methylformamide	6	Hexamethylphosphortriamide	150	Methyl methanesulfonate	5	Ethanesulfonic acid	120	Trimethylphosphite	4	DMSO	70	Acetone	3	Hexafluoroacetone sesquihydrate	68	Dimethyl carbamoyl chloride	3	<i>N</i> -Methyl-2-pyrrolidinone	58	Acetonitrile	3	<i>N,N</i> -Dimethylacetamide	33	Acetic anhydride	3	DMF	27	Trifluoroacetic acid	3	Tetramethylurea	26	Acetic acid	1	Dimethyl methylphosphonate	22	Hexamethyldisilazane	Less than 1	<i>N,N</i> -Dimethylpropionamide	16	Trifluoroacetic anhydride	Less than 1	Bis(dimethylamino) phosphochloridate	14	Hexafluorobenzene	Less than 1	Gamma butyrolactone	14	Pentafluoropyridine	Less than 1	Conc. nitric acid	14	Perfluoro-2-butyltetrahydrofuran	Less than 1
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Solvent	Solubility (ppm)	Solvent	Solubility (ppm)
3-Methylsulfolane	13		
Pyridine	12	Basic solvents:	
Trimethylphosphate	11	Tetramethylguanidine	485
Dimethylcyanamide, vinyl sulfone	8	Bu ₄ NOH, 25% in MeOH	390
Methyl dichlorophosphate		<i>N,N,N,N'</i> -Tetramethylglycinamide	67

Practically insoluble in all common organic solvents^[20], soluble in some superacids^[20]

Solubility in selected solvents, *T* not reported^[20]:

Solvent	Solubility (ppm)
Methanesulfonic acid	820
Hexamethylphosphoric triamide	150
Ethanesulfonic acid	120
DMSO	100
Hexafluoroacetone sesquihydrate	68
<i>N</i> -Methyl-2-pyrrolidinone	58
<i>N,N</i> -Dimethylacetamide	27
DMF	26

Solubility in sulfuric acid/water mixtures, max. quantities of TATB dissolved^[20]:

Acid (vol. %)	<i>g</i> TATB/100 mL solvent
50	< 0.02
66.7	< 0.02
80	0.24
85	0.32
87.5	> 1.28
90	3.84
100	> 24.0

Insoluble or poorly soluble in most common organic solvents^[73], soluble in DMF in presence of inorganic base (e.g. NaOH/KOH)^[73], insoluble in DMF in presence of inorganic base^[73], insoluble in 6 M aq. NaOH soln. @ RT^[73], max. solubility of PG-TATB (production grade) in alkaline DMSO = 25 g/L @ 303 K^[73], soluble in sulfuric acid^[76], 32 mg/L in H₂O @ 25 °C^[84]

Solubility, ppm @ 298.15 K^[76]: 820 in methanesulfonic acid, 150 in hexamethylphosphortriamide, 120 in ethanesulfonic acid, 70 in DMSO, 68 in hexafluoroacetone sesquihydrate, 58 in *N*-methyl-2-pyrrolidinone, 33 in *N,N*-dimethylacetamide, 27 in DMF, 26 in tetramethylurea, 22 in dimethyl methylphosphonate, 16 in *N,N*-dimethyl propionamide, 14 in conc. nitric acid, 13 in 3-methylsulfone, 12 in pyridine, 11 in trimethylphosphate, 3 in acetone, 1 in CH₃CN, acetic anhydride, 1 in trifluoroacetic acid, acetic acid^[76]

Solubility in aqueous sulfuric acid^[76]:

H ₂ SO ₄ :H ₂ O	Acid (vol.%)	g TATB/100 mL H ₂ O
1:1	50	> 0.02
2:1	66.7	< 0.02
7:1	87.5	> 1.28
Conc.	100	> 24.0

Soluble in nitrobenzene and aniline^[79], insoluble in EtOH, Et₂O, CHCl₃, benzene, and glacial acetic acid^[79], nearly insoluble in water, EtOH, Et₂O, benzene, CHCl₃ or glacial acetic acid^[85], soluble in aniline, strong sulfuric acid or nitrobenzene^[85]

Solubility of TATB in sulfuric acid:water mixtures^[85]:

H ₂ SO ₄ :H ₂ O	Acid (vol.%)	Maximum amount dissolved (g TATB/100 mL)
1:1	50	> 0.02
2:1	66.7	< 0.02
4:1	80	~ 0.24
5.67:1	85	~ 0.32
7:1	87.5	> 1.28
9:1	90	~ 3.84
Concentrated	100	> 24.0

"It's unlikely to find a common organic solvent in which TATB is more soluble than 0.1% (w/v)"; exceptions are the superacids in which TATB solubility is >20% (w/v)^[86]

Data (estimated from absorbance measurements) from^[86]:

Solvent	Solubility (ppm)	Solvent	Solubility (ppm)
Methanesulfonic acid	820	<i>N</i> -Methylformamide, tetrahydrofuran (uninhibited)	6
Hexamethylphosphoramide	150	Methyl methanesulfonate	5
Ethanesulfonic acid	120	Trimethylphosphite	4
DMSO	70	Acetone	3
Hexafluoroacetone sesquihydrate	68	Dimethyl carbamoyl chloride	3
<i>N</i> -Methyl-2-pyrrolidinone	58	Acetonitrile	3
<i>N</i> , <i>N</i> -Dimethylacetamide	33	Acetic anhydride	3
DMF	27	Trifluoroacetic acid	3
Tetramethylurea	26	Acetic acid	1
Dimethyl methylphosphonate	22	Hexamethyldisilazane	< 1
<i>N,N</i> -Dimethylpropionamide	16	Trifluoroacetic anhydride	< 1
Bis(dimethylamino) phosphochloridate	14	Hexafluorobenzene	< 1
Gamma butyrolactone	14	Pentafluoropyridine	< 1
Conc. nitric acid	14	Perfluoro-2-butyltetrahydrofuran	< 1
3-Methylsulfolane	13	Water	< 1
Pyridine	12	MeOH	< 1
Trimethylphosphate	11		
Dimethylcyanamide, vinyl sulfone	8		
Methyl dichlorophosphate	7		

Apparent solubility of TATB in basic solvents^[86]:

Solvent	Solubility, ppm
Ethylenediamine	2,195
Tetramethylguanidine	485
Bu ₄ NOH, 25% in MeOH	390
<i>N,N,N',N'</i> -Tetramethylglycinamide	67

Solubility >20% (w/v) in conc. sulfuric acid^[86], chlorosulfonic acid^[86], fluorosulfonic acid^[86] and trifluoromethanesulfonic acid^[86]

Solubility of TATB (g/100 g solvent) after 5 min stirring^[90]:

Solvent	25 °C	98 °C
Dimethylsulfoxide	< 0.1	0.5
<i>N</i> -Methylpyrrolidone	< 0.1	0.8
Aniline	< 0.1	
Sulfuric acid	14	18
Trifluoroacetic acid	< 0.1	

0.16 g/L in H₂O @ 298.15 K (est., Klopman method)^[101], 0.197 g/L in H₂O @ 298.15 K (est., COSMOtherm)^[101]

Hygroscopicity

Effect of oven drying of TATB samples, average % moisture content of TATB after drying at 100 °C^[85]:

Process	Drying time (h)			
	0	24	48	72
Water-aminated	3	0.12	0.09	0.06
Dry-aminated	2.9	0.12	0.09	0.06
Emulsion-aminated	0.16	0.10	0.09	0.09

Moisture content of TATB mixtures^[85]:

Sample	Total moisture content (wt. %)
TATB/Kel-F (90/10)	< 0.0021
TATB/Estane (94/6)	0.0102
TATB/Viton A (91/9)	0.0165

Photosensi- tivity	Yellow solid which turns slightly green on exposure to light which then turns brown on prolonged exposure to sunlight or UV radiation ^[19] , turns green on exposure to sunlight of UV, with prolonged exposure turns brown-black ^[20]																																																		
Radiation sensitivity	<p>Effects of gamma radiation on TATB^[19, 85]:</p> <table><tr><th>Amount of cobalt 60 radia- tion R</th><th>Density before irradiation in g/cm³</th><th>Density after kv irradiation in g/cm³</th><th>Detona- tion velocity in m/s</th><th>Detona- tion pressure in kbar</th><th>Explosion T in °C</th></tr><tr><td>Control</td><td>1.84</td><td>–</td><td>7,510</td><td>260</td><td>403</td></tr><tr><td>1.0 × 10⁷</td><td>1.84</td><td>1.84</td><td>7,520</td><td>260</td><td>394</td></tr><tr><td>9.0 × 10⁷</td><td>1.85</td><td>1.84</td><td>7,525</td><td>261</td><td>370</td></tr><tr><td>7.4 × 10⁸</td><td>1.82</td><td>1.81</td><td>7,435</td><td>250</td><td>345</td></tr></table> <p>Data from^[85]: TATB is yellow but turns green on exposure to radiation from visible, UV, electromagnetic, gamma or ⁶⁰Co sources. Green discoloration is caused by formation of an electronically excited state rather than by a new chemical species (i.e. decomposition product). Shades of green from yellow-green to deep green or brown-green-black have been observed^[85]</p> <p>Data from^[104]:</p> <table><tr><th rowspan="2">Exposure rate (R/h)</th><th rowspan="2">Total dose (R)</th><th>Vacuum stability test</th></tr><tr><th>200 °C (cc/2 g/2 h)</th></tr><tr><td rowspan="5">6.4 × 10⁵</td><td>Control</td><td>0.41</td></tr><tr><td>1.0 × 10⁷</td><td>0.46</td></tr><tr><td>9.0 × 10⁷</td><td>0.57</td></tr><tr><td>7.4 × 10⁸</td><td>0.96</td></tr><tr><td>2.8 × 10⁹</td><td>4.65</td></tr></table>						Amount of cobalt 60 radia- tion R	Density before irradiation in g/cm ³	Density after kv irradiation in g/cm ³	Detona- tion velocity in m/s	Detona- tion pressure in kbar	Explosion T in °C	Control	1.84	–	7,510	260	403	1.0 × 10 ⁷	1.84	1.84	7,520	260	394	9.0 × 10 ⁷	1.85	1.84	7,525	261	370	7.4 × 10 ⁸	1.82	1.81	7,435	250	345	Exposure rate (R/h)	Total dose (R)	Vacuum stability test	200 °C (cc/2 g/2 h)	6.4 × 10 ⁵	Control	0.41	1.0 × 10 ⁷	0.46	9.0 × 10 ⁷	0.57	7.4 × 10 ⁸	0.96	2.8 × 10 ⁹	4.65
Amount of cobalt 60 radia- tion R	Density before irradiation in g/cm ³	Density after kv irradiation in g/cm ³	Detona- tion velocity in m/s	Detona- tion pressure in kbar	Explosion T in °C																																														
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DTA for irradiated explosives @ 20 °C/min^[104]:

Total dose (R)	Exotherms	
	First	
	Onset (°C)	Peak (°C)
0	325	384
1.0×10^7	340	377
9.0×10^7	320	372
7.4×10^8	305	369
2.8×10^9	300	363

TGA for irradiated explosives^[104]:

Total dose (R)	Heating rate (°C/min)	Weight (mg)	Start of dec (°C)	10% weight loss T (°C)	Total weight loss (%)	Remarks
0	20	9.6	285	353	83 @ 420 °C	–
1.0×10^7	20	6.9	280	341	80 @ 400 °C	–
9.0×10^7	20	8.8	250	327	80 @ 385 °C	–
7.4×10^8	20	9.6	250	329	77 @ 405 °C	–
2.8×10^9	20	8.6	125	303	52 @ 345 °C	Detonated @ 345 °C
7.0×10^9	20	8.3	125	299	52% @ 342 °C	Detonated @ 342 °C

Effect of gamma radiation on the mpt. and color^[104]:

Total dose (R)	mpt. (°C)	Color
0	400 dec.	Yellow
1.0×10^7	400 dec.	Yellow green
9.0×10^7	400 dec.	Green
7.4×10^8	400 dec.	Dark green
2.8×10^9	400 dec.	Blackish green

IS for irradiated explosives, 50% fire height in inches, Bruceton method (P.A. apparatus, 2 kg mass)^[104]:

Total Co ⁶⁰ gamma dose (R)	\bar{X} mean (in)	σ std. dev. (in)
0	22.16	3.19
1.0×10^7	17.6	1.28
9.0×10^7	18.39	0.93
7.4×10^8	17.1	3.12

Effect of gamma radiation on explosion T (5 s explosion T in °C) and activation energy (kcal/mol)^[104]:

Total dose (R)	5 s explosion T (°C)	Apparent activation energy (kcal/mol)
0	403	19.30
1.0×10^7	394	18.91
9.0×10^7	370	16.18
7.4×10^8	345	29.28

Effect of gamma radiation on rates of detonation^[104]:

Total dose (R)	Density (g/cc)	Density after irradiation (g/cc)	Rate of detonation (m/s)	Detonation pressure (kbar)
0	1.84	—	7,510	260
1.1×10^7	1.84	1.84	7,520	260
1.3×10^8	1.85	1.84	7,525	261
1.1×10^9	1.82	1.81	7,435	250

Compatibility

Influence of humidity and exposure time on the SSA (specific surface area) of nano-TATB^[40]:

Period (days)	Relative humidity (%)				
	93	76	65	33	12
0	20.4	20.4	20.4	20.4	20.4
25	16.0	16.2	17.0	19.6	20.7
123	14.3	—	14.1	17.2	20.3
175	14.3	—	—	16.5	20.2
250	14.8	—	—	15.8	20.2

	<p>Data from^[85]: A detectable exothermic reaction occurs between TATB and Cu, Fe or Zn at temperatures between 400 and 500 °C in DTA/TGA with a 40 °C/min heating rate. Iron accelerates the TATB dec. rate more than Cu or Zn does, while Al and SiO₂ do not affect the rate^[85].</p> <p>TATB mixtures with three binders (i) Estane 5702-F1, (ii) Kel-F 800 or (iii) Viton A were maintained at 120 °C for 1, 2 or 4 months. Physical changes were observed but no significant chemical changes were detected using chemical analyses. The mixtures with Estane and Viton A were concluded to be suitable for long-term service, however the formulation with Kel-F 800 was not conclusively determined to show long-term stability^[85].</p> <p>Data from^[85]: “coupon” tests on TATB and X-0290 in close proximity to stainless steel, Al, uranium alloys and similar materials showed the metals underwent some corrosion but suffered no effects from the chlorine impurities. Stress and strain were greater at higher test temperatures. The coupon stacks were placed in sealed canisters and aged for 6, 12 and 18 months at elevated temperatures. The canisters were gas-sampled using CRT and the samples tested for mechanical strength at the end of the test series. The test temperatures were in the 50–100 °C range^[85]</p>																										
Dipole moment [D]	0.78 (calcd.) ^[56]																										
Minimum priming charge test [mg]	<p>>15,300 (LANL)^[43]</p> <p>Results of minimum-priming tests, (primer XTX-8003 = PETN/Sylgard (80/20) @ density = 1.53 g cm⁻³) data from^[85]:</p> <table><tr><th rowspan="2">Explosive</th><th rowspan="2">Density (g/cm³)</th><th colspan="2">Amount of XTX</th><th rowspan="2">Result</th></tr><tr><th><i>g</i></th><th>L95</th></tr><tr><td>TATB/HMX/Estane, 2/95/3</td><td>1.840</td><td>0.023</td><td>± 0.093</td><td>Detonation</td></tr><tr><td rowspan="2">TATB/Kel-F 800, 90/10</td><td rowspan="2">1.920</td><td>4.825</td><td></td><td>No detonation</td></tr><tr><td>5.012</td><td></td><td>No detonation</td></tr></table> <p>Minimum priming charge data from^[20]:</p> <table><tr><th>Density (g/cm³)</th><th><i>W</i>₆₀ (mg of XTX 8003)</th><th>Remarks</th></tr><tr><td>1.876</td><td>> 1.53 × 10⁴</td><td>Pressed charge</td></tr></table>	Explosive	Density (g/cm ³)	Amount of XTX		Result	<i>g</i>	L95	TATB/HMX/Estane, 2/95/3	1.840	0.023	± 0.093	Detonation	TATB/Kel-F 800, 90/10	1.920	4.825		No detonation	5.012		No detonation	Density (g/cm ³)	<i>W</i> ₆₀ (mg of XTX 8003)	Remarks	1.876	> 1.53 × 10 ⁴	Pressed charge
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Wedge test

Values with * indicate 30°-wedge, max. thickness = 3.10 cm^[50]:

Sheet no	Brass thickness (cm)	Initial shock velocity of H.E. (m/s)	Initial particle velocity (m/s)	Initial shock pressure H.E. (kbar)	Initial compression H. E. (V/V ₀)	ρ ₀ H.E. (g cm ⁻³)	D (final) (m/s)
1	2.54	4,612	976	83.7	0.788	1.862	Failed to detonate
2	1.27	5,140	1,140	109.1	0.778	1.862	
3	1.27	5,200	1,129	109.3	0.783	1.863	
4*	1.27	5,200	1,129	106.0	0.783	1.800	6,200

Data from^[85]:

Density (g/cm ³)	Initial shock parameters				Coordinates for high-order detonation	
	P ₀ (kbar)	U _{p0} (km/s)	U _{s0} (km/s)	1/2b (km/s)	x* (mm)	t* (μs)
1.876	67.4	0.858	4.186	0.049	<< 12.65	<< 2.92
1.876	94.2	1.063	4.723	0.111	≥ 12.74	≥ 2.44
1.876	130.3	1.340	5.184	0.425	5.80	1.02
1.876	162.2	1.471	5.879	0.684	3.23	0.52

Hugoniot parameters for TATB^[85]:

Initial density (g/cm ³)	Pressure (GPa)	Velocity		Distance to detonation (mm)	Time to detonation (μs)
		U _s shock (km/s)	U _p particle (km/s)		
Standard-grind TATB using plane-wave booster					
1.806	9.42	4.675	1.116	5.37	1.02
1.806	7.95	4.465	0.985	6.54	1.33
1.806	5.12	3.770	0.752	19.6	4.82
1.806	3.34	3.215	0.575	> 25.4	> 8.0

	Superfine TATB using short-duration-shock flyer and wedge																
	1.801	17.4	5.8	1.66	1.77	0.283											
	1.801	22.9	6.2	2.04	1.23	0.222											
	Standard-grind undried TATB using wedge																
	1.84	12.9			3.0	0.54–0.55											
	Pure TATB using wedge																
	1.842	9.0			6.9	1.40											
	1.842	11.8			3.8	0.72											
	Explosive drive, streak camera wedge experiment: distance to detonation = 5.6–0.5 mm for 10–28 GPa pressures ^[85]																
	Data from ^[20] :																
	<table><tr><th>Density (g/cm³)</th><th>Distance, x^* and time t^* to detonation (mm and μs)</th><th>Pressure range (GPa)</th></tr><tr><td>1.714</td><td>$\log P = (1.09 \pm 0.02) - (0.41 \pm 0.17) \log x^*$ $\log P = (0.8 \pm 0.07) - (0.32 \pm 0.12) \log t^*$</td><td>$3.27 < P < 5.64$</td></tr><tr><td>1.841</td><td>$\log P = (1.39 \pm 0.07) - (0.52 \pm 0.07) \log x^*$ $\log P = (1.01 \pm 0.02) - (0.46 \pm 0.05) \log t^*$</td><td>$5.93 < P < 16.5$</td></tr><tr><td>1.876</td><td>$\log P = (1.42 \pm 0.02) - (0.40 \pm 0.03) \log x^*$ $\log P = (1.11 \pm 0.01) - (0.36 \pm 0.03) \log t^*$</td><td>$11.4 < P < 16.22$</td></tr></table>					Density (g/cm ³)	Distance, x^* and time t^* to detonation (mm and μ s)	Pressure range (GPa)	1.714	$\log P = (1.09 \pm 0.02) - (0.41 \pm 0.17) \log x^*$ $\log P = (0.8 \pm 0.07) - (0.32 \pm 0.12) \log t^*$	$3.27 < P < 5.64$	1.841	$\log P = (1.39 \pm 0.07) - (0.52 \pm 0.07) \log x^*$ $\log P = (1.01 \pm 0.02) - (0.46 \pm 0.05) \log t^*$	$5.93 < P < 16.5$	1.876	$\log P = (1.42 \pm 0.02) - (0.40 \pm 0.03) \log x^*$ $\log P = (1.11 \pm 0.01) - (0.36 \pm 0.03) \log t^*$	$11.4 < P < 16.22$
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where P = pressure in GPa																	
Thermal conductivity [cal cm ⁻¹ s ⁻¹ °C ⁻¹]	1.3×10^{-3} ^[20] , 0.00191 ^[58] , 5.4×10^{-3} W m ⁻¹ K ⁻¹ ^[67] , 8.0×10^{-3} J/cm s °C ^[76] , 1×10^{-3} cal/cm s °C ^[99] Thermal conductivity (10^{-4} cal/s-cm-°C) ^[85] : 10.55, $\rho = 1.8268$ g/cm ³ ^[85] , 11.1, $\rho = 1.849$ g/cm ³ ^[85] , 13.0, $\rho = 1.892$ g/cm ³ (LANL) ^[85] , 19.1 (20 °C) ^[85] , 12.4 (100 °C, LLNL) ^[85] , 9.12 (100 °C, LLNL) ^[85] , 6.09 (150 °C, LLNL) ^[85] , 14.2 (160 °C) ^[85] , 12.80 ($\rho = 1.891$ g/cm ³ @ 38 °C, pressed into cylinder) ^[85]																
Specific heat [cal/g-°C]	0.26 ^[58]																

Log K_{ow}	0.7 ^[84] , −1.5 (est., Bruto method) ^[101] , −0.44 (est., Ghose) ^[101] , 4.74 (est. COSMOtherm) ^[101]																																																												
Coefficient of thermal expansion [10 ^{−6} mm/mm-°C]	<p>Thermal expansion of TATB occurs mainly along the <i>c</i>-axis, the relative expansion along the <i>c</i>-axis is ~ 40 × that along the <i>a</i>-axis and 12 × that along the <i>b</i>-axis^[85], volumetric expansion is ~ 3 × that of the linear expansion^[85]</p> <p>Data from^[85]:</p> <table><tr><th>Crystal form</th><th>Measurement</th><th><i>T</i> range (°C)</th><th>Linear expansion</th></tr><tr><td>Triclinic</td><td>X-ray diffraction</td><td>214–377</td><td>101</td></tr><tr><td>Monoclinic</td><td>X-ray diffraction</td><td>216–380</td><td>95</td></tr><tr><td>Powdered compact, $\rho = 1.866 \text{ g/cm}^3$</td><td>Dilatometer</td><td>223–343</td><td>50</td></tr><tr><td rowspan="2">Single crystal</td><td></td><td>0 – −10</td><td>66</td></tr><tr><td></td><td>40–70</td><td>125</td></tr><tr><td rowspan="2">Micronized</td><td></td><td>−50 – −10</td><td>110</td></tr><tr><td></td><td>40–70</td><td>142</td></tr></table>							Crystal form	Measurement	<i>T</i> range (°C)	Linear expansion	Triclinic	X-ray diffraction	214–377	101	Monoclinic	X-ray diffraction	216–380	95	Powdered compact, $\rho = 1.866 \text{ g/cm}^3$	Dilatometer	223–343	50	Single crystal		0 – −10	66		40–70	125	Micronized		−50 – −10	110		40–70	142																								
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Short-shock detonation and Hugoniot experiments	<p>Short-shock detonation and Hugoniot experiments with TATB^[85]:</p> <table><tr><th rowspan="2">Explosive</th><th rowspan="2">Flyer velocity (km/s)</th><th rowspan="2">Pulse duration (ns)</th><th rowspan="2">Pressure (GPa)</th><th colspan="2">Velocity</th><th rowspan="2">Distance to detonation (mm)</th><th rowspan="2">Time to detonation (μs)</th></tr><tr><th>Shock (km/s)</th><th>Particle (km/s)</th></tr><tr><td rowspan="4">TATB standard grind</td><td></td><td></td><td>9.42</td><td>4.675</td><td>1.116</td><td>5.37</td><td>1.02</td></tr><tr><td></td><td></td><td>7.95</td><td>4.465</td><td>0.985</td><td>6.54</td><td>1.33</td></tr><tr><td></td><td></td><td>5.27</td><td>3.913</td><td>0.746</td><td>22.7</td><td>5.38</td></tr><tr><td></td><td></td><td>3.34</td><td>3.125</td><td>0.575</td><td>> 25.4</td><td>> 8.0</td></tr><tr><td rowspan="2">TATB superfine (averages)</td><td>2.62</td><td>170</td><td>17.4</td><td>5.8</td><td>1.66</td><td>1.77</td><td>0.283</td></tr><tr><td>3.26</td><td>74</td><td>22.9</td><td>6.2</td><td>2.04</td><td>1.23</td><td>0.222</td></tr></table>							Explosive	Flyer velocity (km/s)	Pulse duration (ns)	Pressure (GPa)	Velocity		Distance to detonation (mm)	Time to detonation (μs)	Shock (km/s)	Particle (km/s)	TATB standard grind			9.42	4.675	1.116	5.37	1.02			7.95	4.465	0.985	6.54	1.33			5.27	3.913	0.746	22.7	5.38			3.34	3.125	0.575	> 25.4	> 8.0	TATB superfine (averages)	2.62	170	17.4	5.8	1.66	1.77	0.283	3.26	74	22.9	6.2	2.04	1.23	0.222
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Gas-gun experiments	Superfine TATB (@ 1.80 g cm ^{−3}), embedded manganin gauges: distance to detonation = ~ 10 mm with 7.65 GPa input shock ^[85]																																																												
Electrical breakdown voltage [V/mm]	5,750 (pressed TATB) ^[85]																																																												
Skid test	Unreactive ^[85] , TATB/HMX formulations with > 40% TATB did not react ^[85]																																																												
Sled test	No reaction @ velocity <152 mm/s ^[85]																																																												

Cylinder test	LLNL cylinder-test data from ^[85] :					
	Formulation	Density		R-R ₀ (mm)	Velocity (km/s)	
		g/cm ³	% TMD		Wall	Detonation
	TATB	1.800	92.88	5	1.2828	7.478
				19	1.4674	
		1.860		5	1.49	7.76
	Data from ^[20] :					
	Density (g/cm ³)		Cylinder wall velocity (mm/μs) @			
			R-R ₀ = 5 mm		R-R ₀ = 19 mm	
		1.860		1.268		1.446
Cook-off test	Pressed TATB @ 1.73 g cm ⁻³ (90% TMD), cook-off time = 300 s, cook-off temperature = 590 °C, fracture scenario of metal case = ruptured in lids, cook-off reaction = combustion ^[88]					
USA Small-Scale Cookoff Bomb test (SCB test)	Flake TATB, loose fill, heater voltage = 220, cook-off temperature = 388 °C, cook-off time = 2.8 min, cook-off reaction = deflagration ^[89]					
Bullet impact test	Pressed TATB @ 1.73 g cm ⁻³ (90% TMD), bullet caliber = 7.82 mm, bullet velocity = 741 m/s, fracture scenario of metal case = not ruptured, reaction type = no reaction ^[88]					
Jet sensitivity test	Pressed TATB @ 1.70 g cm ⁻³ (90% TMD), critical jet characteristics: X50 (steel plate thickness) = 47.5 mm, V _j (jet velocity) = 5.0 mm/μs, d (jet diameter) = 1.9 mm, V _j ² d = 47.5 mm ³ /μm ² ^[88]					
BIC test	<dp/dt> = 7.2 psi/μs, <E> = 10.7 J/g ^[95]					
Refractive index	TATB crystals are pleochroic (colorless parallel to x-axis, yellow in y-z plane) ^[20]					

ODTX data from^[91]:

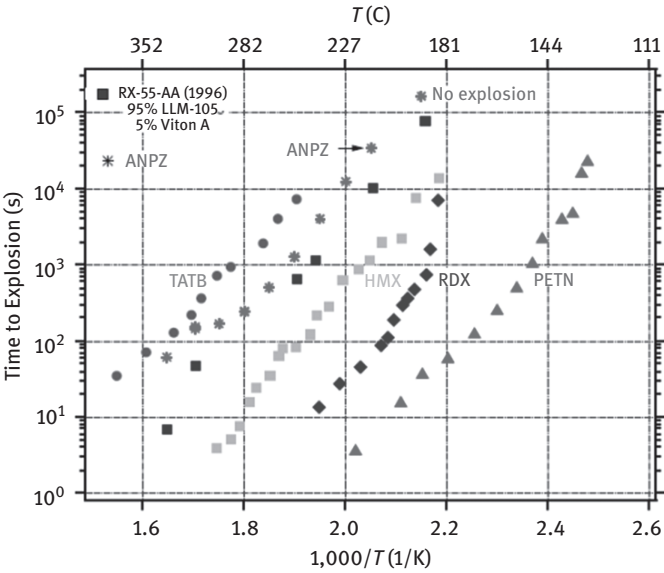


Fig. 18: ODTX results of ANPZ and TATB, HMX, RDX and PETN^[91].

	TATB ^[4, 19, 20, 22, 72, 76, 85]	TATB ^[27, 85]	TATB ^[27, 85]
Chemical formula	C ₆ H ₆ N ₆ O ₆	C ₆ H ₆ N ₆ O ₆	C ₆ H ₆ N ₆ O ₆
Molecular weight [g mol ⁻¹]	258.15	258.15	258.15
Crystal system	Triclinic	Monoclinic	Triclinic
Space group	P-1 (no. 2)		
<i>a</i> [Å]	9.010 ± 0.003	13.386(3)	4.599(1)
<i>b</i> [Å]	9.028 ± 0.003	9.039(3)	6.541(2)
<i>c</i> [Å]	6.812 ± 0.003	8.388(2)	7.983(1)
α [°]	108.59 ± 0.02	90	103.81(2)
β [°]	91.82 ± 0.03	118.75(2)	92.87(1)
γ [°]	119.97 ± 0.01	90	116.95(2)
<i>V</i> [Å ³]	442.524	889.803	204.374
<i>Z</i>	2		
ρ_{calc} [g cm ⁻³]	1.937		
<i>T</i> [K]	295	295	295

Measured cell constants for triclinic form TATB at various temperatures, data from^[27]:

$T(^{\circ}\text{C})$	$a(\text{\AA})$	$b(\text{\AA})$	$c(\text{\AA})$	$\alpha(^{\circ})$	$\beta(^{\circ})$	$\gamma(^{\circ})$	Volume (\AA^3)	No. of reflections
-59 ± 3	9.007(4)	9.023(3)	6.713(3)	108.75(4)	92.03(4)	119.98(3)	434.5	13
-45 ± 3	9.013(5)	9.032(4)	6.727(5)	108.78(5)	91.96(6)	119.99(4)	436.2	13
-36 ± 1	9.007(3)	9.029(3)	6.734(3)	108.74(3)	92.04(3)	119.97(2)	436.3	13
-26 ± 1	9.007(4)	9.033(3)	6.748(2)	108.75(2)	91.98(3)	119.96(3)	437.4	13
-13 ± 3	9.007(4)	9.030(3)	6.762(2)	108.64(3)	92.04(3)	119.93(3)	438.7	13
-1 ± 1	8.989(5)	9.033(5)	6.776(6)	108.69(7)	92.07(7)	119.90(4)	438.8	13
11 ± 2	9.015(3)	9.033(3)	6.797(2)	108.66(2)	91.88(2)	119.96(2)	441.6	13
23 ± 1	9.017(5)	9.031(3)	6.815(2)	108.63(3)	91.90(3)	119.95(3)	442.9	13
35 ± 1	9.018(4)	9.047(3)	6.856(5)	108.39(5)	92.04(5)	119.95(3)	447.0	10
44 ± 1	9.014(3)	9.045(5)	6.857(7)	108.43(7)	92.04(4)	119.94(3)	446.7	10
54 ± 1	9.016(2)	9.046(6)	6.872(6)	108.49(7)	91.97(4)	119.95(4)	447.7	10
65 ± 1	9.016(5)	9.049(4)	6.891(9)	108.40(7)	91.99(8)	119.93(4)	449.5	10
76 ± 1	9.015(5)	9.050(4)	6.923(8)	108.41(7)	91.97(7)	119.89(4)	451.9	10
83 ± 1	9.019(5)	9.054(3)	6.943(6)	108.41(5)	91.99(6)	119.90(4)	453.4	10
94 ± 1	9.014(6)	9.052(4)	6.963(8)	108.39(7)	91.96(8)	119.87(5)	454.7	10
104 ± 1	9.016(8)	9.054(5)	6.980(9)	108.39(8)	91.90(10)	119.86(6)	456.2	10
$23 \pm 1^*$	9.019(2)	9.033(4)	6.810(3)	108.54(5)	91.96(3)	119.98(3)	442.8	10

* Determined after low- and high-temperature data

Measured cell constants for *C*-centered monoclinic form of TATB at various temperatures, data from^[27]:

$T(^{\circ}\text{C})$	$a(\text{\AA})$	$b(\text{\AA})$	$c(\text{\AA})$	$\beta(^{\circ})$	Volume (\AA^3)	No. of reflections
-57 ± 1	13.217(4)	9.034(2)	8.313(2)	118.15(2)	875.2	12
-47 ± 3	13.217(5)	9.028(3)	8.312(3)	118.19(2)	874.1	12
-34 ± 2	13.249(3)	9.027(3)	8.329(3)	118.27(2)	877.3	12
-23 ± 2	13.267(4)	9.030(3)	8.335(2)	118.38(2)	878.5	12
-12 ± 1	13.278(3)	9.031(3)	8.344(1)	118.39(1)	880.2	12
1 ± 1	13.313(4)	9.032(2)	8.359(2)	118.52(2)	883.0	12

12 ± 1	13.344(4)	9.034(2)	8.369(2)	118.64(2)	885.5	12
23 ± 1	13.386(3)	9.039(3)	8.388(2)	118.75(2)	889.8	12
35 ± 1	13.431(7)	9.049(4)	8.418(7)	118.97(4)	895.1	12
45 ± 1	13.456(9)	9.043(5)	8.433(8)	119.10(6)	896.7	12
57 ± 2	13.498(10)	9.042(6)	8.442(9)	119.24(6)	899.1	12
67 ± 1	13.514(9)	9.048(7)	8.453(7)	119.30(5)	901.4	12
76 ± 1	13.540(10)	9.041(7)	8.466(9)	119.39(6)	903.0	12
86 ± 1	13.590(19)	9.049(9)	8.476(7)	119.38(7)	908.3	12
95 ± 1	13.702(10)	9.022(20)	8.523(15)	120.16(10)	910.9	12
107 ± 1	13.713(20)	9.055(9)	8.534(12)	119.94(9)	918.2	12
23 ± 1*	13.365(18)	9.044(7)	8.380(5)	118.91(7)	886.8	12

Cell constants between 214 and 377 K show a volume change of +5.1%^[19], expansion is almost entirely due to a 4% increase in the *c* axis^[19]

Cell parameters of TATB undergoing thermal cycling process from 30 to 240 °C and from 240 to 30 °C, XRD data, particle size ~ 20 µm, >99% purity^[72]:

<i>T</i> (°C)	<i>a</i> (Å)	<i>b</i> (Å)	<i>c</i> (Å)	α (°)	β (°)	γ (°)	Volume (Å ³)
30	9.016	9.033	6.827	108.68	91.77	119.97	443.70
60	9.022	9.037	6.860	108.64	91.73	119.97	446.66
90	9.020	9.034	6.888	108.61	91.69	119.98	448.40
120	9.025	9.041	6.925	108.58	91.66	119.97	451.63
150	9.029	9.042	6.959	108.55	91.61	119.98	454.29
180	9.029	9.047	6.993	108.55	91.56	119.98	456.91
210	9.035	9.051	7.033	108.52	91.53	119.99	460.08
240	9.036	9.049	7.068	108.53	91.50	119.97	462.43
240	9.036	9.052	7.067	108.54	91.49	120.01	462.36
210	9.037	9.051	7.031	108.52	91.54	119.99	460.12
180	9.034	9.049	6.995	108.56	91.56	119.98	457.35
150	9.028	9.044	6.962	108.57	91.59	119.98	454.49
120	9.023	9.039	6.922	108.60	91.63	119.97	451.22
90	9.019	9.035	6.890	108.60	91.67	119.99	448.52
60	9.021	9.038	6.861	108.65	91.71	119.98	446.63
30	9.015	9.032	6.827	108.68	91.76	119.97	443.67

Exptl. determined cell volumes of TATB (Triclinic and Monoclinic forms) from 214 to 377 K XRD data^[76]:

Triclinic form		C-centered monoclinic form	
<i>T</i> (°C)	Vol (Å ³)	<i>T</i> (°C)	Vol (Å ³)
−59 ± 3	434.5	−57 ± 1	875.2
−45 ± 3	436.2	−47 ± 2	874.1
−36 ± 1	436.3	−34 ± 2	877.3
−26 ± 1	437.4	−23 ± 2	878.5
−13 ± 3	438.7	−12 ± 1	880.2
11 ± 2	441.6	1 ± 1	883.0
23 ± 1	442.9	12 ± 1	885.5
35 ± 1	447.0	23 ± 1	889.8
44 ± 1	446.7	35 ± 1	895.1
54 ± 1	447.7	45 ± 1	896.7
65 ± 1	449.5	57 ± 2	899.1
76 ± 1	451.9	67 ± 1	901.4
83 ± 1	453.4	76 ± 1	903.0
94 ± 1	454.7	86 ± 1	908.3
104 ± 1	456.2	95 ± 1	910.9

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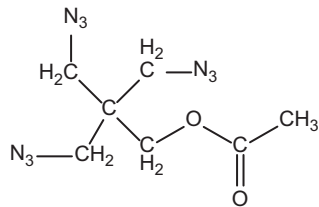
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Triazidopentaerythrite-acetate

Name [German, acronym]: Triazidopentaerythrite-acetate [TAP-Ac]

Main (potential) use: Potential new plasticizer^[1, 2]

Structural formula:



	TAP-Ac		
Formula	C ₇ H ₁₁ N ₉ O ₂		
Molecular mass [g mol ⁻¹]	253.23		
Appearance at RT			
IS [J]	1 Nm ^[1] , H ₅₀ = 29.9 cm (2 kg mass, 30 mg sample) ^[2]		
FS [N]	54 ^[1] , 8% (66° swing angle, 2.45 MPa) ^[2]		
N [%]	49.78		
Ω(CO ₂) [%]	-110.57		
T _{glass transition} [°C]	-86 – -83 ^[1] , -73.86 ^[2]		
T _{dec.} [°C]	241.36 (DSC, peak max) ^[1] , 208 (onset), 251.9 (exo peak max) (DSC @ 10 °C/min) ^[2]		
ρ [g cm ⁻³]	1.244 ^[1] , 1.25 ^[2]		
Heat of formation			
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
-Δ _{ex} U° [kJ kg ⁻¹]			
T _{ex} [K]			
p _{C-J} [kbar]			
VoD [m s ⁻¹]			

V_0 [L kg ⁻¹]			
Refractive index, η_D^{20}	1.5092 ^[1]		

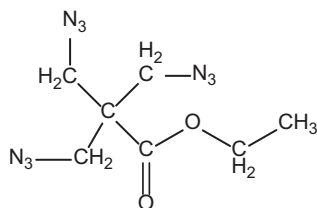
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Triazidopivalic-acid-ethylester

Name [German, acronym]: Triazidopivalic-acid-ethylester [TAPE-E]

Main (potential) use: Potential new plasticizer^[1]

Structural formula:



	TAPE-E		
Formula	C ₇ H ₁₁ N ₉ O ₂		
Molecular mass [g mol ⁻¹]	253.23		
Appearance at RT	Pale yellow oil ^[1]		
IS [J]	1 Nm ^[1]		
FS [N]	64 ^[1]		
N [%]	49.78		
Ω(CO ₂) [%]	-110.57		
T _{glass transition} [°C]	-94 – -92 ^[1]		
T _{dec.} [°C]	221.76 (DSC, peak max) ^[1]		
ρ [g cm ⁻³]	1.218 ^[1]		
Heat of formation			
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
-Δ _{ex} U° [kJ kg ⁻¹]			
T _{ex} [K]			
p _{C-J} [kbar]			
VoD [m s ⁻¹]			
V ₀ [L kg ⁻¹]			
Refractive index, η _D ²⁰	1.4990 ^[1]		

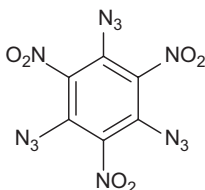
[1] G. Unkelbach, T. Keicher, H. Krause, *Synthesis and Characterization of New Triazido-Plasticizers*, ICT **2005**, Karlsruhe, Germany, pp. 49-1-49-8.

1,3,5-Triazido-2,4,6-trinitrobenzene

Name [German, acronym]: Trinitro-triazidobenzene, triazidotrinitrobenzol [TATNB, TNTAB]

Main (potential) use: Initiating explosive, high explosive in compound detonators^[15], ingredient of primer mix^[6, 16], priming compositions^[17]

Structural formula:



	TATNB																																																		
Formula	$C_6N_{12}O_6$																																																		
Molecular mass [g mol ⁻¹]	336.14																																																		
Appearance at RT	Greenish-yellow crystals ^[6, 15, 16] , bright yellow crystals ^[13] , bright yellow solid ^[14] , greenish-yellow solid ^[17]																																																		
IS [J]	<p><4.9 (≤25 cm, 2 kg mass, 20 mg sample, B.M.)^[6], explodes if 250 g mass dropped from 60 cm^[2], explodes if 5 kg mass dropped from 60 cm^[2], 25 cm (2 kg mass, B.M.)^[11, 17], FI = 6% of PA^[11], $H_{60\%}$ = 30 cm (Wöhler apparatus)^[11], 2.5 (50% prob., 500 g hammer, 50 cm)^[13], 2 (0% prob., 2 kg hammer)^[13], 3.9 (100% prob., 2 kg hammer)^[13], 5 (ignition)^[13], >1.5 (250 g hammer, 60 cm)^[13]</p> <p>Influence of grit on IS^[19]:</p> <table border="1"> <thead> <tr> <th rowspan="2">Grit</th><th rowspan="2">Hardness (mols.)</th><th rowspan="2">mpt. (°C)</th><th colspan="2">Explosion efficiency (45 g, 30 cm)</th></tr> <tr> <th>No.</th><th>%</th></tr> </thead> <tbody> <tr> <td>Nil</td><td>–</td><td>–</td><td>0/15</td><td>0</td></tr> <tr> <td>Silver nitrate</td><td>2–3</td><td>212</td><td>0/5</td><td>0</td></tr> <tr> <td>Silver bromide</td><td>2–3</td><td>434</td><td>0/5</td><td>0</td></tr> <tr> <td>Lead nitrate</td><td>2–3</td><td>470</td><td>0/10</td><td>0</td></tr> <tr> <td>Lead chloride</td><td>2–3</td><td>501</td><td>2/20</td><td>10</td></tr> <tr> <td>Borax</td><td>3–4</td><td>560</td><td>5/5</td><td>100</td></tr> <tr> <td>Bismuthinite</td><td>2–2.5</td><td>685</td><td>5/5</td><td>100</td></tr> <tr> <td>Chalcocite</td><td>3–3.5</td><td>1,100</td><td>5/5</td><td>100</td></tr> </tbody> </table>				Grit	Hardness (mols.)	mpt. (°C)	Explosion efficiency (45 g, 30 cm)		No.	%	Nil	–	–	0/15	0	Silver nitrate	2–3	212	0/5	0	Silver bromide	2–3	434	0/5	0	Lead nitrate	2–3	470	0/10	0	Lead chloride	2–3	501	2/20	10	Borax	3–4	560	5/5	100	Bismuthinite	2–2.5	685	5/5	100	Chalcocite	3–3.5	1,100	5/5	100
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Chalcocite	3–3.5	1,100	5/5	100																																															

ESD [J]	Explodes if subjected to ESD of 20 kv ^[2]		
N [%]	50.00		
$\Omega(\text{CO}_2)$ [%]	−28.56		
$T_{\text{m.p.}}$ [°C]	131 ^[1, 13, 17] , 131 (dec.) ^[6, 11, 15] , 128–130 (dec.) ^[2] , 130 (dec.) ^[18] , melting can occur at T as low as 120 °C if the sample is kept for 6 min at this T ^[18]		
ρ [g cm ^{−3}]	1.80 (@ 293 K) ^[1] , 1.81 (crystal) ^[6] , 1.805 (crystal) ^[11] , 1.75 (pressed @ 42,000 psi) ^[6, 11] , 1.7509 (@ 3,000 kg/cm ²) ^[11] , 1.7526 (@ 5,000 kg/cm ²) ^[11] , 1.805 (pycnometric) ^[13] , 1.84 (X-ray) ^[13] , sp. gr. = 1.8054 (crystals) ^[15] , 1.7509 (blocks under 3,000 kg/cm ² pressure) ^[15] , 1.7526 (blocks under 5,000 kg/cm ² pressure) ^[15]		
Heat of formation	765.8 kJ/mol ($\Delta_f H^\circ$) ^[2] , 270 kcal/mol ^[7] , 2,278.0 kJ/kg ($\Delta_f H^\circ$) ^[2]		
Heat of combustion	$\Delta H_c = -3,232$ kJ/mol (Parr bomb calorimeter) ^[2] , 840 kcal/mol (Q_c^V) ^[11] , 2,254 cal/g ^[6, 11, 12] , 3,200 kJ/mol (exptl.) ^[13]		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^\circ$ [kJ kg ^{−1}]	6,195		5,397 [H ₂ O (g)] ^[9]
T_{ex} [K]	4,912	4,600 (@ 1.74 g cm ^{−3} , calcd. BKWR) ^[7] 5,640 (@ 1.74 g cm ^{−3} , calcd. BKWS) ^[7]	
$p_{\text{C-J}}$ [kbar]	355	18.4 GPa (calcd., K-J) ^[2] 321 (@ 1.74 g cm ^{−3} , calcd. BKWR) ^[7] 312 (@ 1.74 g cm ^{−3} , calcd. BKWS) ^[7]	
VoD [m s ^{−1}]	9,065 (@ 1.80 g cm ^{−3})	8,100 (calcd., K-J) ^[2] 7,200 (@ 1.50 g cm ^{−3}) ^[13] 7,500 (@ 1.54 g cm ^{−3}) ^[13] 8,100 (@ 1.70 g cm ^{−3}) ^[13] 8,440 (@ 1.74 g cm ^{−3} , calcd. BKWR) ^[7] 8,390 (@ 1.74 g cm ^{−3} , calcd. BKWS) ^[7]	8,100 ^[2] 8,580 (@ 1.74 g cm ^{−3}) ^[3, 5, 7] 9,030 (@ 1.81 g cm ^{−3}) ^[4] 7,300 (@ 1.71 g cm ^{−3}) ^[10]
V_0 [L kg ^{−1}]	739		755 ^[8]

Trauzl test [cm ³ , % TNT]	179% TNT (@ 1.0 g cm ⁻³) ^[11] , 165–171% TNT ^[11] , 150% TNT ^[13] , 179% TNT ^[13] , 90% PETN ^[6, 15, 17]																																									
Ballistic mortar test	147% TNT ^[11]																																									
Initiation efficiency	0.02 g for TNT (TNT pressed @ 49 MPa) ^[13] , 0.01 g for Tetryl (Tetryl pressed @ 49 MPa) ^[13] , 1 g TNT compressed in No. 8 detonator shell under pressure of 500 kg/cm ² with TATNB compressed on top of it under 300 kg/cm ² required 0.62 g of TATNB for complete detonation ^[15] , did not explode when initiated unconfined in thin layers by hot wire ^[19]																																									
Dead-pressing	Dead-pressed @ ~ 42,000 psi ^[6] , brisance rapidly decreases @ pressures >29 MPa ^[13] , dead-pressed @ 290 MPa ^[13]																																									
5 s explosion <i>T</i> [°C] 10 s explosion <i>T</i> [°C] 10 s ignition <i>T</i> [°C]	150 ^[6] 150 ^[11, 13] 150 ^[12]																																									
Thermal stability	<div>Dependence of weight loss of TATNB on temp. and time^[13]:</div> <table><tr><th><i>T</i> (°C)</th><th>Time (days)</th><th>Weight loss (%)</th><th><i>T</i> (°C)</th><th>Time (days)</th><th>Weight loss (%)</th></tr><tr><td rowspan="5">20</td><td>~ 50</td><td>~ 0</td><td rowspan="4">35</td><td>~ 25</td><td>~ 0.2</td></tr><tr><td>~ 190</td><td>~ 0.1</td><td>~ 75</td><td>~ 1</td></tr><tr><td>~ 400</td><td>~ 0.2</td><td>~ 250</td><td>~ 2</td></tr><tr><td>~ 590</td><td>~ 0.4</td><td>~ 625</td><td>~ 4.4</td></tr><tr><td>~ 900</td><td>~ 0.6</td><td rowspan="4">50</td><td>~ 25</td><td>~ 0.5</td></tr><tr><td>~ 1,050</td><td>~ 0.8</td><td>~ 50</td><td>~ 0.2</td></tr><tr><td>~ 1,150</td><td>~ 0.9</td><td>~ 150</td><td>~ 9.5</td></tr><tr><td></td><td></td><td>~ 200</td><td>~ 13</td></tr></table> <div>Complete dec. observed after 14 h @ 100 °C^[13], 0.665% dec. in 3 years @ 20 °C^[15], 2.43% dec. in 1 year @ 35 °C^[15], 0.65% dec. in 10 days @ 50 °C^[15], 100% dec. in 14 h @ 100 °C^[15]</div>	<i>T</i> (°C)	Time (days)	Weight loss (%)	<i>T</i> (°C)	Time (days)	Weight loss (%)	20	~ 50	~ 0	35	~ 25	~ 0.2	~ 190	~ 0.1	~ 75	~ 1	~ 400	~ 0.2	~ 250	~ 2	~ 590	~ 0.4	~ 625	~ 4.4	~ 900	~ 0.6	50	~ 25	~ 0.5	~ 1,050	~ 0.8	~ 50	~ 0.2	~ 1,150	~ 0.9	~ 150	~ 9.5			~ 200	~ 13
<i>T</i> (°C)	Time (days)	Weight loss (%)	<i>T</i> (°C)	Time (days)	Weight loss (%)																																					
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~ 1,050	~ 0.8	~ 50		~ 0.2																																						
~ 1,150	~ 0.9	~ 150		~ 9.5																																						
		~ 200		~ 13																																						
Volatility	Not appreciably volatile @ 35–50 °C ^[15]																																									
Burn rate [mm/s]	0.65 cm/s ^[6] , 0.03 (0.5 mm thick layer) ^[13] , 0.05 (single crystal) ^[13] , burns with greenish flame ^[15] , 3 cm/s (unconfined) ^[19]																																									

Solubility [g/mL]	Qualitative solubilities at room temperature ^[6] :	
	Solvent	Solubility
	Acetone	Readily soluble
	Chloroform	Moderately soluble
	Alcohol	Sparingly soluble
	Water	Insoluble
	Soluble in acetone, benzene ^[13] , slightly soluble in alcohols ^[13, 16] , insoluble in H ₂ O ^[13, 15, 16] , readily soluble in acetone ^[15] , moderately soluble in CHCl ₃ ^[15, 16] , sparingly soluble in EtOH ^[15] , readily soluble in acetone ^[16] , can be recryst. from CHCl ₃ ^[6]	
Hygroscopicity	0.00% @ 30 °C with 90% RH ^[6] , nonhygroscopic ^[13, 15] , absorbs 1.35 wt. % H ₂ O within 40 days exposure to moist air (slightly hygroscopic) ^[13] , nonhygroscopic ^[17]	
Photosensitivity	Light sensitive ^[13] , darkens superficially on exposure to light ^[15]	
Compatibility	Wet TATNB does not attack Fe, steel or copper ^[6] , quantitative dec. in boiling acetic acid ^[14] , does not react with common metals such as Fe, steel, Cu or brass ^[17] , stable in H ₂ O: no change in 3.5 years under H ₂ O ^[13]	

	TATNB^[2]
Chemical formula	C ₆ N ₁₂ O ₆
Molecular weight [g mol ⁻¹]	336.18
Crystal system	Monoclinic
Space group	<i>P</i> 2 ₁ / <i>c</i>
<i>a</i> [Å]	5.4256(4)
<i>b</i> [Å]	18.5515(13)
<i>c</i> [Å]	12.1285(10)
α [°]	90
β [°]	94.907(10)
γ [°]	90
<i>V</i> [Å ³]	1,216.30(16)
<i>Z</i>	4
ρ_{calc} [g cm ⁻³]	1.836
<i>T</i> [K]	200

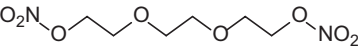
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Triethyleneglycol dinitrate

Name [German, acronym]: Triethylene glycol dinitrate, 2,2-ethylenedioxydiethyl-dinitrate, dinitroethylene glycol, nitrotriglycol, dinitrotriglycol, triglycol dinitrate [triglykoldinitrat, TEGN, TEGDN]

Main (potential) use: Ingredient of double-base propellants, rocket propellants^[5, 7, 17], component of liquid explosives,^[10] gelatinizing agent for NC in propellants,^[10] plasticizer in pyrotechnic flares^[10], plasticizer in fabrication of flexible explosive sheets^[10], best plasticizing ability toward NC amongst the polyhydric alcohols^[22]

Structural formula:



	TEGN
Formula	C ₆ H ₁₂ N ₂ O ₈
Molecular mass [g mol ⁻¹]	240.17
Appearance at RT	Light yellow, oily liquid ^[8, 10] , oily liquid ^[13, 22]
IS [J]	100 + cm (2 kg mass, 20 mg sample, B.M.) ^[5, 17] , 43 in (2 kg mass, P.A.) ^[5, 17] , 12.7 Nm ^[7] , 100 cm (2 kg mass) ^[6] , >100 cm (20 mg sample, B.M.) ^[8] , 43 in (P.A.) ^[8] , 43 in (P.A., 1 lb mass) ^[9] , >100 cm (B.M.) ^[10] , 109 cm (P.A.) ^[10] , 100 cm (2 kg mass, B.M.) ^[9] , 100 cm ^[15] , 66 cm (median height, Rotter apparatus) ^[19] , 100 cm (2 kg dropping hammer) ^[22]
FS [N]	Unaffected by steel shoe (friction pendulum test) ^[5, 8, 10] , unaffected by fiber shoe (friction pendulum test) ^[5, 8, 10]
N [%]	11.66
Ω(CO ₂) [%]	-66.62
T _{m.p.} [°C]	-40 ^[6] , -19 ^[8, 10, 15, 17] (commercial products with DEGDN impurities freeze @ -57 °C) ^[9] , -23 ^[21] , -40 (freezing point) ^[22]
T _{dec.} [°C]	195 (DSC @ 5 °C/min), ~ 110 (onset, DSC) ^[16]
ρ [g cm ⁻³]	1.344 (@ 293 K) ^[1] , 1.348 (@ 293 K) ^[4] , 1.33 (@ 20 °C) ^[5, 9] , 1.32 (@ 25 °C) ^[5] , 1.335 ^[8, 10, 22] , sp. gr. = 1.335 ^[13] , d ₁₆ ¹⁶ = 1.3291 ^[14] , 1.33 ^[15, 21] , d ₁₆ ¹⁶ = 1.3291 ^[22]

Heat of formation	$-656.9 \text{ kJ/mol } (\Delta_f H^\circ (\text{s}))^{[2]}$, $-603.8 \text{ kJ/mol } (\Delta_f H^\circ (\text{s}))^{[2]}$, $-2,619 \text{ kJ/kg}$ (enthalpy of form., ICT thermochemical database) ^[3, 7] , $-654 \text{ cal/g}^{[4]}$, $-181.6 \text{ kcal/mol } (\Delta H_f, @ 25^\circ \text{C})^{[9]}$, $-576.6 \text{ kcal/kg } (@ \text{C}^\vee)^{[8]}$, $-603.7 \text{ kcal/kg } (@ \text{C}^\text{p})^{[8]}$, $-603.7 \text{ kcal per mol}^{[10]}$, $-2,619 \text{ J/g } (\Delta H_f)^{[15]}$, -629 kJ/mol (enthalpy of form.) ^[21] , $-99.4 \text{ kcal/mol}^{[23]}$, -656.9 kJ/mol (enthalpy of form., exptl.) ^[24] , -605.8 kJ/mol (enthalpy of form., calcd., emp.) ^[24]		
Heat of combustion	$3,428 \text{ kcal/kg}^{[5, 11]}$, $3,428 \text{ cal/g } (@ 18 \text{ mm})^{[8]}$, $819.2 \text{ kcal/mol } (@ \text{ constant pressure})^{[8]}$, $836.60 \text{ kcal/mol } (Q_c^\vee, \text{ liq. H}_2\text{O})^{[8]}$, $\Delta H_c = 14,343 \text{ J/g}^{[15]}$, $3,428 \text{ cal/g } (@ \text{C}^\text{p})^{[10]}$, $\Delta_c H^\circ (\text{l}) = -3,440 \text{ kJ/mol}^{[2]}$, $\Delta_c H^\circ (\text{l}) = -3,500.4 \text{ kJ/mol}^{[2]}$		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{\text{ex}} U^\circ [\text{kJ kg}^{-1}]$	4,177	$357 \text{ kcal/kg}^{[11]}$ 750 kcal/kg (heat of det.) ^[13] $3,317 \text{ J/g}$ (calcd., ICT-code) ^[3] $3,318 \text{ J/g } (\Delta H_\theta)^{[15]}$ 3.14 MJ/kg (heat of explosion) ^[18] $3,320 [\text{H}_2\text{O} (\text{l})]^{[21]}$ $3,138$ (heat of explosion) ^[22] $2,510.4$ (explosion heat @ constant volume) ^[22]	$357 \text{ cal/g}^{[5]}$ $3,138 \text{ J/g}^{[6]}$ $2,629 \text{ J/g}$ (of constant volume) ^[6] $3,317 [\text{H}_2\text{O} (\text{l})]^{[7]}$ $750 \text{ cal/kg } (@ \text{ const. pressure})^{[8]}$ $725 \text{ kcal/kg}^{[10]}$
$T_{\text{ex}} [\text{K}]$	2,880	$2,025$ (calcd., ICT-code) ^[3] $2,100^{[22]}$	$2,100^{[6]}$
$p_{\text{C-J}} [\text{kbar}]$	16.3	102.5 MPa (calcd., ICT-code) ^[3] 189 (@ 1.38 g cm^{-3} , calcd. BKWR) ^[23] 183 (@ 1.38 g cm^{-3} , calcd. BKWS) ^[23]	

VoD [m s ⁻¹]	6,608	7,080 (@ 1.38 g cm ⁻³ , calcd. BKWR) ^[23] 7,190 (@ 1.38 g cm ⁻³ , calcd. BKWS) ^[1]	Fails (@ 1.33 g cm ⁻³ , 1.25 in charge diameter, liquid, Shelby steel confinement) ^[5] No detonation (@ 1.44 g cm ⁻³ , rel. light steel tubing, 3.175 cm diameter) ^[10] <2,000 (heavily confined) ^[10] <2,000 (under heavy confinement, ρ not specified) ^[8] No. det. under mild confinement (steel, @ 1.33 g cm ⁻³ , diameter = 1.25 in) ^[8] 6,760 (@ 1.38 g cm ⁻³) ^[23]
V ₀ [L kg ⁻¹]	837	1,214 mL/g [H ₂ O (l)]	1,065 ^[7] 851 ^[5]
Trauzl test [cm ³ , % TNT]	320 cc ^[8, 20, 22]		
Sand test [g]	14.7 g sand crushed (200 g bomb, cf. 48.0 g for TNT) ^[5, 8] , 14.7 g (30.6% TNT, 200 g bomb) ^[10] , 14.7 g (200 g bomb) ^[17]		
5 s explosion T [°C] Explosion T [°C] 5 s ignition T [°C] Deflagration T [°C]	223 ^[5, 17] , 225 ^[10] , 225 (0.02 g sample) ^[8] 245 ^[22] 223 ^[11] , 225 ^[8] 195 ^[8, 10]		
100 °C heat test [% mass loss]	1.8% mass loss in first 48 h (0.6 g sample) ^[5, 8, 10] , 1.6% mass loss in second 48 h @ 100 °C (0.6 g sample) ^[5, 8, 10] , no explosions in test period (0.6 g sample) ^[5, 8, 10]		
Vacuum stability test [cm ³ /h]	0.45 cc/40 h @ 100 °C ^[5] , 0.8 cc/16 h @ 120 °C ^[5] , 45 mL gas evolved in 40 h @ 100 °C ^[10] , 0.8–0.99 mL gas evolved in 8 h @ 120 °C ^[10] @ 100 °C: 0.45 cc/40 h ^[8] , 0.7–0.9 cc/g/8 h ^[8]		
Vapor pressure [atm. @ °C]	<0.001 mm Hg @ 25 °C ^[5, 8, 10]		
Volatility	40 mg/cm ² /h @ 60 °C ^[5, 8, 10] , lower than NG ^[15] , 1/5 th –1/6 th NG value ^[22]		

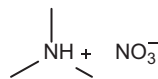
Viscosity [cP]	<p>13.2 Poises (@ 20 °C)^[5, 8, 10], 0.257 Poises @ 6.0 °C^[14], 0.119 Poises @ 20.3 °C^[14], 0.015 Poises @ 54.2 °C^[14], 2.5 times that of NG @ 20 °C^[22]</p> <p>Viscosity values (no units given) from^[22]:</p> <table border="1"> <tr> <th>T (°C)</th><th>Viscosity, η</th></tr> <tr> <td>6.0</td><td>0.257</td></tr> <tr> <td>20.3</td><td>0.119</td></tr> <tr> <td>54.2</td><td>0.015</td></tr> </table>	T (°C)	Viscosity, η	6.0	0.257	20.3	0.119	54.2	0.015
T (°C)	Viscosity, η								
6.0	0.257								
20.3	0.119								
54.2	0.015								
Solubility [g/mL]	<p>0.55 g/100 g H₂O @ 25 °C^[5], 0.68 g/100 g H₂O @ 60 °C^[5], 0.7 g/100 g H₂O @ 20 °C^[22], soluble in Et₂O, acetone, acetic acid^[22], insoluble in EtOH^[22]</p> <p>TEGN has a high plastic solubility for NC^[22]</p> <p>Solubility (g/100 g solvent) at 25 °C^[5]: Et₂O = w^[5], alcohol = ∞^[5], 2:1 ether:alcohol = w^[5], acetone = w^[5], very soluble in acetone, Et₂O, Et₂O/EtOH (2:1)^[10], soluble in CS₂^[10], slowly soluble in water^[10], 7,400 mg/L H₂O @ 25 °C^[12], very soluble in acetone, ether, 2:1 Et₂O/EtOH^[8], soluble in CS₂^[8], slightly soluble in water^[8]</p>								
Hygroscopicity	0.144 @ relative humidity of 65, similar to DEGN ^[22]								
Compatibility	Hydrolysis: 10 days @ 22 °C, 0.032% acid ^[5] , 5 days @ 60 °C, 0.029% acid ^[5]								
Refractive index	$n_{20}^D = 1.4540$ ^[5, 10] , $n_D^{21.2} = 1.4542$ ^[22]								
Batch sorption experiments	$K_{ow} = 6.23 \pm 0.11$ ^[12] , K_d (DRDC-08) = 0.09 ± 0.03 L/kg ^[12] , K_d (WCL) = 0.78 ± 0.08 L/kg ^[12]								
Abel test	>40 min @ 72 °C ^[22]								

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Trimethylammonium nitrate

Name [German, acronym]: Trimethylamine nitrate [trimethylaminnitrat, TMAN]
Main (potential) use: Component in castable charges^[3]
Structural formula:



	Trimethylammonium nitrate		
Formula	C ₃ H ₁₀ N ₂ O ₃		
Molecular mass [g mol ⁻¹]	122.12		
Appearance at RT			
N [%]	22.94		
Ω(CO ₂) [%]	−104.81		
T _{phase transition} [°C]	86, 136 (DTA, Al cups, atm. pressure) ^[5] , 90, 134 (DTA, Al cups, 0.5 mm Hg pressure) ^[5]		
T _{m,p.} [°C]	428 K ^[1] , 153 ^[4] , 157 ^[4] , DSC (Pt cups, atm. pressure): 86 (endo), 136 (endo), 157 (endo), 202 (exo) ^[5] , DSC (Pt cups, 0.5 mm Hg pressure): 90 (endo), 134 (endo), 155 (endo), 163 (exo) ^[5]		
T _{dec.} [°C]	DSC (Pt cups, atmospheric pressure): 202 (exo) ^[5] , DSC (Pt cups, 0.5 mm Hg pressure): 163 (exo) ^[5] , TG inflection point = 186 (weight loss = 97%) ^[5]		
ρ [g cm ⁻³]	1.25–1.28 ^[1] , 1.50 ^[3]		
Heat of formation	−343.6 kJ/mol (enthalpy of form., exptl.) ^[2] , −313.0 kJ/mol (enthalpy of form., calcd.) ^[2] , −2,816.2 kJ/kg (enthalpy of form.) ^[3] , −562 kcal/kg (energy of form.) ^[4] , −598 kcal/kg (enthalpy of form.) ^[4]		
	Calcd. (EXPLO5 5.04)	Lit. values	Exptl.
−Δ _{ex} U° [kJ kg ⁻¹]	3,428	834 kcal/kg (Q _e) ^[4]	2,140 [H ₂ O (l)] ^[3]
T _{ex} [K]	2,144		
p _{C-J} [kbar]	144		
VoD [m s ⁻¹]	6,841 (@ 1.23 g cm ⁻³ , Δ _f H = −313 kJ mol ⁻¹)		
V ₀ [L kg ⁻¹]	977	1,102 (on det.) ^[4]	1,244 ^[3]

5 s explosion T [°C] Initiation T [°C]	202 (deflagration) ^[4]
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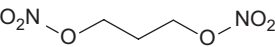
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Trimethyleneglycol dinitrate

Name [German, acronym]: Trimethyleneglycol dinitrate, 1,3-propanediol dinitrate, 1,3-propylene glycol dinitrate, nitropropylene glycol [trimethylenglykoldinitrat]

Main (potential) use: Initiating explosive

Structural formula:



	Trimethyleneglycol dinitrate		
Formula	C ₃ H ₆ N ₂ O ₆		
Molecular mass [g mol ⁻¹]	166.09		
Appearance at RT	Oily liquid ^[5, 8] , water-white very mobile liquid ^[7]		
IS [J]	100 cm (2 kg mass) ^[4] , 100 cm (2 kg mass) fails to initiate explosion ^[5, 8]		
N [%]	16.87		
Ω(CO ₂) [%]	−28.90		
T _{b,p.} [°C]	180 (@ 10 mm Hg) ^[5, 8] , 180 (@ 10 mm Hg, without dec.) ^[7]		
T _{dec.} [°C]	225 (DSC @ 5 °C/min)		
ρ [g cm ⁻³]	1.4053 (@ 289 K) ^[1] , 1.393 (@ 20 °C) ^[4] , sp. gr. = 1.393 (@ 20 °C) ^[5, 8] , d ¹⁶ ₁₆ = 1.4053 ^[6] , d ₄ ²⁰ = 1.3952 ^[6] , sp. gr. (20°/4°) = 1.393 @ 20 °C ^[7]		
Heat of formation	−224.0 kJ/mol (Δ _f H°) ^[2]		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
−Δ _{ex} U° [kJ kg ⁻¹]	5,587	1,138.5 kcal/kg [H ₂ O (vapor)] ^[5] 4,763.5 (explosion heat) [H ₂ O vapor] ^[8]	4,763.5 J/g [H ₂ O (g)] ^[4]
T _{ex} [K]	3,854		
p _{C-J} [kbar]	212		
VoD [m s ⁻¹]	7,373		7,340 (@ 1.5 g cm ⁻³) ^[3]
V ₀ [L kg ⁻¹]	863		

Trauzl test [cm ³ , % TNT]	540 cc (~90% NG, 10 g sample, H ₂ O tamping) ^[5, 7, 8] , 470 cm ³ (93% blasting gelatin cf. 80% that of NG blasting gelatin) ^[8]
5 s explosion <i>T</i> [°C] Explosion <i>T</i> [°C]	225 ^[5, 8] , ~ 225 (deflagrates on slow heating) ^[7]
Thermal stability	No dec. @ 75 °C for 25 days ^[5] , no dec. after heating at 75 °C for 600 h ^[8]
Volatility	Higher than that of NG ^[8]
Solubility [g/mL]	Miscible with same solvents as NG ^[5]
Viscosity [P]	$\eta_{20} = 5.8$ cP ^[6] , 0.0940 @ 6.3 °C ^[6] , 0.0550 @ 20.2 °C ^[6] , 0.0275 @ 54.2 °C ^[6] , lower than that of NG ^[8]
Dielectric constant, ϵ_{20}	18.97 ^[6]

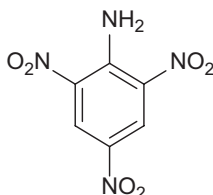
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Trinitroaniline

Name [German, acronym]: 2,4,6-Trinitroaniline, 1-amino-2,4,6-trinitrobenzene, picramide [picramid, TNA]

Main (potential) use: High-temperature heat-resistant explosive^[8]

Structural formula:



	TNA
Formula	$C_6H_4N_4O_6$
Molecular mass [g mol ⁻¹]	228.12
Appearance at RT	Yellow ^[8] , deep yellow crystals ^[27] , orange-red crystals ^[28, 42] , yellow needle-like solid ^[30] , yellow crystalline ^[44]
IS [J]	23 in (2 kg mass, 20 mg sample, P.A.) ^[8] , 15 Nm ^[13] , log $H_{50\%} = 2.25$ ^[11] , 35.25 ^[12] , $H_{50} = 177$ cm ^[14, 30] , $H_{50\%} = 177$ cm ^[16, 26] , FI = 111% PA ^[17] , FI = 122% PA ^[17] , 50% point = 36 cm (10 kg mass, French method) ^[17] impact work for 50% explosions = 10.4 kg/cm ² (2 kg mass) ^[17] , 177 cm ^[30] , $H_{50} = 141$ cm (34.5 J) ^[32] , 177 cm (Bruceton method, type 12 tool, 2.5 kg mass, 40 mg sample, 5/0 sandpaper, 25 trials) ^[33] , 177 cm (2.5 kg mass) ^[36] , 137.8 cm (5 kg mass, AFATL) ^[36] , $H_{50} = 141$ cm (2.5 kg mass, type 12 tool) ^[38] , log(H_{50}) = 2.248 (Kamlet/Adolph) ^[39] , $H_{50\%} = 141$ cm (2.5 kg mass) ^[48]
FS [N]	353 ^[13]
ESD [J]	6.85 ^[5, 12]
N [%]	24.56
Ω(CO ₂) [%]	-56.11
$T_{m.p.}$ [°C]	188 ^[1, 18, 30] , 189–190 ^[8] , 461 K ^[14] , 189–192 ^[17] , 192 ^[19, 40] , 190 ^[28] , 186 ^[28] , 188 (Thomas Hoover Capillary Melting Point Apparatus @ 2 °C/min) ^[35] , 186–188 ^[42] , 192–195 ^[44] , 187–188 ^[49] , 185–189 (crude, lower purity, recryst. from acetone gave mpt. of 188–189 °C) ^[49]
$T_{b.p.}$ [°C]	Dec. before boiling point ^[8]

$T_{\text{dec.}} [^{\circ}\text{C}]$	346 (DSC @ 5 $^{\circ}\text{C}/\text{min}$), 387 (exo peak max., DSC @ 20 $^{\circ}\text{C}/\text{min}$) ^[19]		
$\rho [\text{g cm}^{-3}]$	1.762 (@ 293 K) ^[3, 13] , 1.76 (crystal) ^[8] , 1.76 (@ 20 $^{\circ}\text{C}$) ^[17] , 1.773 (crystal) ^[15] , 1.773 ^[24] , 1.762 (crystal) ^[30] , 1.74 (exptl. ρ) ^[30] , 1.72 (loading ρ @ 50,000 psi) ^[8] , 1.76 ^[47] , 1.760 ^[14]		
Heat of formation	−72.8 kJ/mol ($\Delta_f H^{\circ}(\text{s})$) ^[4] , −115.9 kJ/mol ($\Delta_f H^{\circ}(\text{s})$) ^[4] , 21.6 kcal mol ^{−1} (Q_f average) ^[17] , 131 cal/g ^[8] , −78 cal/g ($\Delta_f H^{\circ}$) ^[14] , −17.4 kcal/mol ($\Delta H_f(\text{s})$) ^[24] , −20.07 kcal/mol ^[30] , −368.1 kJ/kg (ΔH_f , ICT thermochemical database) ^[31] , −78.0 kcal/kg (enthalpy of form.) ^[34] , 57.5 kcal/kg ^[43] , −71.1 kJ/mol (ΔH_f) ^[47]		
Heat of combustion	678 kcal mol ^{−1} (Q_c^{P} average) ^[17] , 680 kcal mol ^{−1} (Q_c^{V} average) ^[17] , heat of combustion = 2,962 cal/g ^[8] , 3,008 kcal/kg (@ $^{\circ}\text{C}$) ^[43] , $\Delta_c H^{\circ}(\text{s})$ = −2,860.1 kJ/mol ^[4] , $\Delta_c H^{\circ}(\text{s})$ = −2,816.87 kJ/mol ^[4]		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{\text{ex}} U^{\circ} [\text{kJ kg}^{-1}]$	4,331	1,018 cal/g ^[23] 1.26 kcal/g (Q_{max} , calcd.) ^[24] 827 cal/g (det. energy) ^[30] 903 cal/g (calcd. det. energy, Q , using ΔH_f values for explosive and dec. products) ^[30] 903 (@ 1.6 g cm ^{−3} , calcd. Halford–Kistiakowsky equation of state) ^[30] 3,589 (calcd., ICT-code) ^[31] 1,023 kcal/kg (@ 1.720 g cm ^{−3} , calcd.) [H ₂ O vapor] ^[34] $-\Delta H_{\text{det}} = 5.24 \text{ kJ/g}$ ^[47]	3,589 [H ₂ O (l)] ^[7, 13] 564 cal/g ^[8] 4.263 kJ g ^{−1} ^[14] 3,488 [H ₂ O (g)] ^[13] 1,019 kcal/kg [H ₂ O (g)] ^[10] 191.2 kcal mol ^{−1} (Q_e) ^[17] 1,019 kcal/kg (@ 1.720 g cm ^{−3}) [H ₂ O vapor] ^[34] 990 kcal/kg ^[44]
$T_{\text{ex}} [\text{K}]$	3,203	2,839 (@ 1.6 g cm ^{−3} , calcd. Halford–Kistiakowsky equation of state) ^[30] 2,663 (calcd., ICT-code) ^[31]	~3,700 $^{\circ}\text{C}$ ^[17]

p_{CJ} [kbar]	225	232 (@ 1.72 g cm ⁻³ , <i>Xiong</i>) ^[23] 251 (@ 1.773 g cm ⁻³ , calcd.) ^[24] 241 (calcd.) ^[30] 179.8 (@ 1.6 g cm ⁻³ , calcd. Halford–Kistiakowsky equation of state) ^[30] 109.6 (calcd., ICT-code) ^[31]	24.7 GPa ^[14]
VoD [m s ⁻¹]	7,442 (@ 1.76 g/cc)	7,490 (@ 1.76 g cm ⁻³ (TMD), calcd., R-P method) ^[22] 7,720 (@ 1.76 g cm ⁻³ (TMD), calcd., <i>Aizenshtadt</i>) ^[22] 7,480 (@ 1.76 g cm ⁻³ (TMD), calcd., K-J) ^[22] 7,373 (@ 1.72 g cm ⁻³ , <i>Xiong</i>) ^[22] 7,550 (@ 1.773 g cm ⁻³ , calcd.) ^[24] 7,440 (@ 1.74 g cm ⁻³) ^[30] 7,055 (@ 1.6 g cm ⁻³ , calcd. Halford–Kistiakowsky eqn. of state) ^[30]	7,300 (@ 1.72 g cm ⁻³ , 0.5 in charge diameter, pressed, no confinement) ^[8] 7,300 (@ 1.72 g cm ⁻³) ^[13, 23, 24] 7,420 (@ 1.76 g cm ⁻³) ^[6] 7,600 (@ 1.7 g cm ⁻³) ^[20] 7,000 (@ 1.5 g cm ⁻³ , compressed TNA in cardboard cartridges, 30 mm diameter, 3 mm thick) ^[17] <i>see additional values in the table at the end of this section</i>
V_0 [L kg ⁻¹]	648	0.4839 cm ³ /g (@ 1.6 g cm ⁻³ , calcd. Halford–Kistiakowsky equation of state) ^[30]	838 ^[9, 13] 724 ^[44]
Critical diameter [cm]	0.3 cm ^[30]		
Trauzl test [cm ³ , % TNT]	107% TNT ^[8, 20] , 92% PA ^[17] , 98% TNT ^[17] , 296 cc ^[44] , 310 ^[46]		
Sand test [g]	48.1 g (200 g bomb) ^[8]		
Ballistic mortar test	100% TNT ^[8]		
Initiation efficiency	0.30 g LA minimum detonating charge ^[8]		
Plate-push value	2,347 ft/s (@ 93% crystal ρ , for TNA/Zytel 95:5 PBX) ^[30]		

SSGT [cm]	<p>4.0 mm (NOL)^[27], P₉₀ = 27.91 kbar (P₉₀ = pressure to 90% of TMD, NSW small-scale gap test)^[33]</p> <p>Picramide, TMD = 1.76, data from^[45]:</p> <table><tr><th>Loading pressure (kpsi)</th><th colspan="2">Density (g/cm³)</th><th>% TMD</th><th colspan="4">Sensitivity (DBG)</th></tr><tr><th></th><th>AVG.</th><th><i>s</i></th><th></th><th>AVG.</th><th><i>g</i></th><th><i>s_m</i></th><th><i>N</i></th></tr><tr><td>4</td><td>1.389</td><td>0.0033</td><td>78.9</td><td>5.549</td><td>0.0173</td><td>0.0169</td><td>20</td></tr><tr><td>8</td><td>1.469</td><td>0.0037</td><td>83.5</td><td>5.941</td><td>0.0218</td><td>0.0183</td><td>20</td></tr><tr><td>16</td><td>1.562</td><td>0.0034</td><td>88.8</td><td>6.470</td><td>0.0173</td><td>0.0167</td><td>20</td></tr><tr><td>32</td><td>1.646</td><td>0.0052</td><td>93.5</td><td>6.985</td><td>0.0320</td><td>0.0255</td><td>20</td></tr><tr><td>64</td><td>1.719</td><td>0.0028</td><td>97.7</td><td>7.783</td><td>0.0370</td><td>0.0324</td><td>20</td></tr></table>	Loading pressure (kpsi)	Density (g/cm ³)		% TMD	Sensitivity (DBG)					AVG.	<i>s</i>		AVG.	<i>g</i>	<i>s_m</i>	<i>N</i>	4	1.389	0.0033	78.9	5.549	0.0173	0.0169	20	8	1.469	0.0037	83.5	5.941	0.0218	0.0183	20	16	1.562	0.0034	88.8	6.470	0.0173	0.0167	20	32	1.646	0.0052	93.5	6.985	0.0320	0.0255	20	64	1.719	0.0028	97.7	7.783	0.0370	0.0324	20									
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Thermal stability	No. moles gas formed per mole TNA/no. h: @ 120 °C: 0/22, 0/72 ^[19] , @ 220 °C: 0.25/22, 0.5/72 ^[19] , @ 320 °C: 3.21/22, 3.41/72 ^[19]																																																																	
Vacuum stability test [cm ³ /h]	0.9 cc/40 h @ 100 °C ^[8] , comparable values to TNT @ 140 °C ^[17] , 0.0 cm ³ /g/48 h @ 100 °C ^[30]																																																																	
Vapor pressure [atm. @ °C]	<p>1.74 × 10⁻⁶ Torr @ 66 °C^[21]</p> <p>Values from^[41]:</p> <table><tr><th><i>T</i> (°C)</th><th>Vapor pressure (x10⁷ Torr)</th><th>Wt. loss (g × 10³)</th><th>Time (s)</th><th>Area (cm²)</th></tr><tr><td>55.7</td><td>5.48</td><td>4.82</td><td>235,080</td><td>0.770</td></tr><tr><td>55.7</td><td>5.37</td><td>4.62</td><td>235,080</td><td>0.753</td></tr><tr><td>55.7</td><td>4.80</td><td>10.60</td><td>322,200</td><td>1.410</td></tr><tr><td>55.7</td><td>4.92</td><td>19.50</td><td>322,200</td><td>2.53</td></tr><tr><td>62.6</td><td>10.80</td><td>13.25</td><td>331,200</td><td>0.770</td></tr><tr><td>62.6</td><td>11.10</td><td>13.84</td><td>331,200</td><td>0.783</td></tr><tr><td>78.2</td><td>68.0</td><td>18.86</td><td>76,680</td><td>0.770</td></tr><tr><td>78.2</td><td>65.6</td><td>18.11</td><td>76,680</td><td>0.766</td></tr><tr><td>78.2</td><td>68.3</td><td>18.54</td><td>76,680</td><td>0.753</td></tr><tr><td>85.3</td><td>163</td><td>125.20</td><td>65,160</td><td>2.53</td></tr><tr><td>97.6</td><td>628</td><td>52.60</td><td>23,760</td><td>0.770</td></tr><tr><td>97.6</td><td>625</td><td>53.19</td><td>23,760</td><td>0.783</td></tr></table>	<i>T</i> (°C)	Vapor pressure (x10 ⁷ Torr)	Wt. loss (g × 10 ³)	Time (s)	Area (cm ²)	55.7	5.48	4.82	235,080	0.770	55.7	5.37	4.62	235,080	0.753	55.7	4.80	10.60	322,200	1.410	55.7	4.92	19.50	322,200	2.53	62.6	10.80	13.25	331,200	0.770	62.6	11.10	13.84	331,200	0.783	78.2	68.0	18.86	76,680	0.770	78.2	65.6	18.11	76,680	0.766	78.2	68.3	18.54	76,680	0.753	85.3	163	125.20	65,160	2.53	97.6	628	52.60	23,760	0.770	97.6	625	53.19	23,760	0.783
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Solubility [g/mL]	Insoluble in water ^[8] , slightly soluble in EtOH and Et ₂ O ^[8] , soluble in hot glacial acetic acid, hot ethyl acetate, in benzene and acetone ^[8] , poorly soluble in EtOH and Et ₂ O ^[27] , soluble in hot acetone, benzene and ethyl acetate ^[27] , recryst. from acetone ^[49]
Hygroscopicity	Hygroscopic ^[44]
Dipole moment [D]	2.31 (calcd.) ^[36]
ΔH_{sub} [kJ/mol]	125.3 (exptl.) ^[37] , 127.0 (calcd., QSPR) ^[37] , 27.71 kcal (molar heat of sublimation) ^[41] , 121.5 cal/g (specific heat of sublimation) ^[41]
Closed cylinder test	Gas pressure by exploding sample in small bomb; pressure measured by piston and obturator: loading $\rho = 0.20 \text{ g cm}^{-3}$, pressure = 2,080 kg/cm ² ^[25, 29] , loading $\rho = 0.25 \text{ g cm}^{-3}$, pressure = 2,885 kg/cm ² ^[25, 29] , loading $\rho = 0.30 \text{ g cm}^{-3}$, pressure = 3,970 kg/cm ² ^[25] , loading $\rho = 0.30 \text{ g cm}^{-3}$, pressure = 3,940 kg/cm ² ^[29]

Detonation velocities of TNA (exptl. values)^[30]:

Charge no.	Diameter (cm)	Length (cm)	Confinement	ρ (g/cm ³)	VoD (m/s)
1 [†]	Conical [‡]	2.34	None	1.726	-
	0.64	1.34	None	1.726	7,345
	1.27	1.34	None	1.746	7,310
	1.27	2.76	None	1.750	7,310
	2.54	2.76	None	1.737	7,560
	2.54	2.74	None	1.746	7,560
	2.54	2.74	None	1.744	7,560
	2.54	2.77	None	1.728	7,560
2	4.43	15.24	Cu	1.485	6,800

[†] charge 1 was in the form of a pyramid consisting of 1 conical and 3 cylindrical sections

[‡] diameter uniformly decreased from 0.63 to 0.32 cm over 2.34 cm length

	TNA ^[3]	TNA ^[15]
Chemical formula	C ₆ H ₄ N ₄ O ₆	C ₆ H ₄ N ₄ O ₆
Molecular weight [g mol ⁻¹]	228.13	228.13
Crystal system	Monoclinic	Monoclinic
Space group	<i>P</i> 2 ₁ / <i>c</i> (no. 14)	<i>P</i> 2 ₁ / <i>c</i> (no. 14)
<i>a</i> [Å]	5.9722(1)	6.137 ± 0.003
<i>b</i> [Å]	9.1789(1)	9.217 ± 0.007
<i>c</i> [Å]	15.2935(2)	15.323 ± 0.007
α [°]	90	90

β [°]	99.073(1)	99.67 ± 0.02
γ [°]	90	90
V [Å ³]	827.87(2)	
Z	4	4
ρ_{calc} [g cm ⁻³]	1.830	1.773
T [K]	100	

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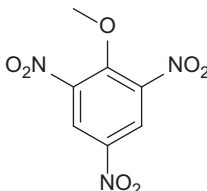
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Trinitroanisole

Name [German, acronym]: Trinitroanisole, 2-methoxy-1,3,5-trinitrobenzene, 2,4,6-trinitroanisole, 2,4,6-trinitrophenylmethylether, methylpicrate, nitrolite, 1-methoxy-2,4,6-trinitrobenzene [piktrinsäuremethylether, TNAN, TNAs]

Main (potential) use: Used to lower the melting points of other explosives but poor stability in presence of moisture, booster charge component, used in World War I as mixture with HNDPS in bombs^[17]

Structural formula:



	Trinitroanisole
Formula	$C_7H_5N_3O_7$
Molecular mass [g mol ⁻¹]	243.13
Appearance at RT	White needles ^[16] , pale yellow leaflets on recryst. from MeOH ^[17] , white crystals separate from anhydrous solvents ^[17] , white crystalline solid (pure) or pale yellow crystalline solid ^[24] , yellow crystals ^[25] , crystalline substance ^[27]
IS [J]	$H_{50} = 192$ cm ^[8] , 48 ^[9] , 20 Nm ^[10] , 15–16 in (2 kg mass, P.A.) ^[11] , 19 cm (max. value for no explosion, 5 kg mass) ^[11] , FI = 120–124% PA ^[11] , 20.20 (drop energy, Julius-Peters app.) ^[12] , $H_{50\%} = 192$ cm ^[13] , less sensitive than PA ^[16] , 124–129% PA ^[16] , $H_{20\%} = 100$ cm (5 kg mass) ^[17] , $H_{30\%} = 110$ cm (5 kg mass) ^[17] , 192 cm (Bruceton method, type 12 tool, 2.5 kg mass, 40 mg sample, 5/0 sandpaper, 25 trials) ^[20] , 79.3 cm (5 kg mass, AFATL) ^[21] , 192 cm (2.5 kg mass) ^[21] , $H_{50} = 192$ cm (2.5 kg mass, type 12 tool) ^[22] , $\log(H_{50}) = 2.283$ (Kamlet/Adolph) ^[23]
FS [N]	353 ^[10]
ESD [J]	28.59 ^[9, 29]
N [%]	17.28
$\Omega(\text{CO}_2)$ [%]	−62.52
$T_{\text{m.p.}}$ [°C]	68 ^[1, 10] , 68.4 ^[11, 27] , 68 (α -TNAs) ^[11] , 57.5 (β -TNAs) ^[11] , 67 ^[16] , 67–68 ^[17, 25] , 66–68 ^[24]

$T_{\text{dec.}}$ [°C]	285 (DSC @ 5 °C/min), 482 K (DTA onset) ^[19]		
ρ [g cm ⁻³]	1.61 ^[2] , 1.408 (molten) ^[10] , 1.4 (cast) ^[11] , 1.7 (@ max. loading pressure) ^[11] , sp. gr. = 1.408 ^[16]		
Heat of formation	-187.2 kJ/mol ($\Delta_f H^\circ$ (s)) ^[3] , -630.1 kJ/kg (enthalpy of form.) ^[10] , 132.0 kcal/kg ^[26]		
Heat of combustion	$\Delta_c H^\circ$ (s) = -3,310.1 ± 3.3 kJ/mol ^[3] , $\Delta_c H^\circ$ = -3,281.93 kJ/mol ^[3] , 792.1 kcal/mol (Q_c^V (average)) ^[11] , 784.4 kcal/mol (Q_c^P (average)) ^[11] , 3,269 kcal/kg (@ C ^V) ^[26]		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{\text{ex}} U^\circ$ [kJ kg ⁻¹]	4,321	4.62 MJ/kg (heat of explosion) ^[28]	3,777 [H ₂ O (l)] ^[5, 10] 2,469 [H ₂ O (g)] ^[7] 3,656 [H ₂ O (g)] ^[10]
T_{ex} [K]	3,284	2,366 (calcd.) ^[11]	
p_{C-J} [kbar]	182		
VoD [m s ⁻¹]	6,720 (@ 1.57 g cm ⁻³)	7,150 (@ 1.59–1.7 g cm ⁻³ , average value from lit.) ^[15] 7,640 (@ 1.60 g cm ⁻³ , max. VoD) ^[16]	6,800 (@ 1.57 g cm ⁻³) ^[10] 6,300 (@ 1.5 g cm ⁻³) ^[7] 6,800 (@ 1.61 g cm ⁻³) ^[4] 6,600 (@ 1.59 g cm ⁻³) ^[11] 7,000 (@ 1.59 g cm ⁻³) ^[15] 7,166 (calcd. based on sand expt.) ^[15]
V_0 [L kg ⁻¹]	670		844 ^[6, 10] 740 ^[27]

Trauzl test [cm ³ , % TNT]	98% PA ^[11] , 112% TNT ^[11] , 104–108% TNT ^[15]
Sand test [g]	110% TNT ^[11] , 100–110% TNT ^[15] , 41.7 g sand crushed (1,700 g bomb) ^[15]
Ballistic mortar test	106% TNT ^[11] , 106–108% TNT ^[15]

Initiation efficiency	Smallest amount of primary explosive necessary (g) to cause detonation of TNA: 0.1 g cadmium azide ^[18] , 0.26 g silver azide ^[18] , 0.28 g LA ^[18] , 0.375 g cuprous azide ^[18] , 0.55 mercurous azide ^[18] , 0.23 g silver fulminate ^[18] , 0.26 g cadmium fulminate ^[18] , 0.32 g copper fulminate ^[18] , 0.37 g mercury fulminate ^[18]
5 s explosion T [°C] Explosion T [°C] 5 s ignition T [°C] Detonating T [°C]	165–296 ^[11] , 225 ^[11] , 279–500 ^[11] 290–296 ^[14] ~165 ^[24]
Thermal stability	No change on heating @ 95 °C for 24 h ^[16]
Solubility [g/mL]	Recryst. from MeOH ^[17] , very poorly soluble in H ₂ O ^[16] , 0.02 g / 100 mL H ₂ O @ 15 °C ^[16] , 0.137 g/100 mL H ₂ O @ 50 °C ^[16] , sparingly soluble in CS ₂ , CCl ₄ ^[16] , soluble in EtOH ^[16] , very soluble in Et ₂ O, benzene, CHCl ₃ and ethyl acetate ^[16] , soluble in benzene, CHCl ₃ , ethyl acetate, acetic acid and acetone ^[24]
Hygroscopicity	Reacts slowly with moisture ^[17] , slightly hygroscopic ^[24]
Compatibility	Reacts slowly with moisture ^[17] , does not react with metals ^[24] , exposure to moisture produces PA which reacts with metals ^[24] , does not react with metals if moisture is not present ^[25]
Dipole moment [D]	2.12 (calcd.) ^[21]
Fugacity	314 cc ^[27]
Manometric bomb	Pressure (max. theoretical) if exploded in own volume and without loss of heat = 9,235 kg/cm ² @ 1.5 g cm ⁻³ ^[11] , 2,145–2,222 kg/cm ² (@ 0.20 g cm ⁻³ , manometric bomb) ^[16, 17] , 2,850 kg/cm ² (@ 0.25 g cm ⁻³ , manometric bomb) ^[16, 17]

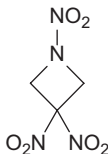
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Trinitroazetidine

Name [German, acronym]: 1,3,3-Trinitroazetidine [trinitroazetidin, TNAZ]
 Main (potential) use: LOVA^[31], melt-castable explosive^[31], explosive suitable for casting alone or as a casting matrix for other explosives^[26], possible application as a castable explosive, plasticizer or “high-energy TNT replacement”^[18]

Structural formula:



	TNAZ
Formula	C ₃ H ₄ N ₄ O ₆
Molecular mass [g mol ⁻¹]	192.09
Appearance at RT	Clear, colorless crystals ^[17] , colorless microcrystalline solid ^[36]
IS [J]	6 Nm ^[5] , 6.90 ^[4] , 21 cm (2.5 kg hammer) ^[9] , $H_{50\%} = 45\text{--}47$ cm (3 kg mass, NOL apparatus) ^[13] , FOI = 110 (rel. to RDX (FOI = 80), Rotter apparatus) ^[12] , 86 cm (2.5 kg, tool type 12A, 35 mg sample, pressed pellets, Gen-Corp Aerojet sample) ^[14] , 29 cm (2.5 kg, tool type 12A, 35 mg pressed pellets, Elgin Air Force Base sample, $\geq 99.8\%$ purity) ^[14] , 28 cm (2.5 kg mass, tool type 12A, 35 mg pressed pellets, recrystallized sample) ^[14] , $H_{50} = 26$ cm (2 kg hammer) ^[23] , $H_{50} = 29$ cm ^[24] , $H_{50} = 26$ cm (2 kg hammer, $E_{d50} = 5.2$ J) ^[28] , $A_{d2} = 10\%$, $LL = 0.7$ m, $A_{50\text{ d}1} = 2.0$ m ^[34]
FS [N]	324 ^[5] , 110 ^[7] , 160 (BAM) ^[12] , 36 kg (NOL apparatus) ^[13] , 5.4 kg (BAM, Gen-Corp Aerojet sample) ^[14] , 8.0 kg (BAM, Elgin Air Force Base sample, $\geq 99.8\%$ purity) ^[14] , 11.6 kg (recrystallized sample) ^[14]
ESD [J]	2.49 ^[4] , 8.76 ^[6] , 78.3 mJ ^[6] , 4.5 ^[12] , 1 J with 510 Ω = no reaction with Gen-Corp Aerojet sample ^[14] , 1 J with 510 Ω = no reaction with Elgin Air Force Base sample, $\geq 99.8\%$ purity ^[14] , 1 J with 510 Ω = no reaction with recrystallized sample ^[14]
N [%]	29.17
$\Omega(\text{CO}_2)$ [%]	-16.66

$T_{m,p}$. [°C]	101 ^[1, 8, 11, 13, 18, 30] , 101 (DSC @ 10 °C/min) ^[13] , 99 (onset, DSC) ^[12] , 99.45 (max. peak, DSC @ 10 °C/min, Gen-Corp Aerojet sample) ^[14] , 99.36 (max. peak, DSC @ 10 °C/min, Elgin Air Force Base sample, ≥99.8% purity) ^[14] , 96.83 (max. peak, DSC @ 10 °C/min, recrystallized sample) ^[14] , 99.4–100.4 (TNAZ purified by sublimation) ^[14] , 99 (DSC @ 10 °C/min, open pan sample) ^[15] , 99 (DSC @ 10 °C/min, pierced pan sample) ^[15] , 99 (DSC @ 10 °C/min, closed pan sample) ^[15] , 103–104 ^[17] , 101 (onset @ 97; max. @ 102, sealed glass capillary, DSC @ 20 °C/min) ^[21] , 105–165 (vaporization, broad peak, DSC (@ 10 °C/min, open pan sample) ^[15] , 145–205 (vaporization, broad peak, DSC (@ 10 °C/min, pierced pan sample) ^[15] , 100.61 (endo, DSC @ 5 °C/min, 9.0 mg sample, hermetic Al pans, Ar atmosphere, first cycle through 30–175 °C) ^[27] , 99.9 (endo peak max, DSC @ 5 K/min, pierced Al pan) ^[18] , 99.5 (endo peak max, DSC @ 5 K/min, sealed Al pan) ^[18] , 100.59 ± 0.21 ^[30] , 101–102 ^[35] , 98–99 (microcrystalline, uncorrected) ^[36] Melting onset T (and peak T) as a function of thermal cycling (TNAZ cycled 40–205 °C) ^[27] : cycle no. 1, mpt. = 98.2 (100.1); cycle no. 2, mpt. = 96 (100) ; cycle no. 3, mpt. = 93.3 (98) ^[27]								
$T_{b,p}$. [°C]	252 ^[30]								
T_{dec} . [°C]	>240 (DSC @ 5 °C/min) ^[2] , 185 (DTA) ^[12] , 232 (onset, DSC @ 10 °C/min, Gen-Corp Aerojet sample) ^[14] , 243 (onset, DSC @ 10 °C/min, Elgin Air Force Base sample, ≥99.8% purity) ^[14] , 245 (onset, DSC @ 10 °C/min, recrystallized sample) ^[14] , 220–290 (DSC @ 10 °C/min, closed pan sample) ^[15] , 278 (exo peak max., DSC @ 20 °C/min) ^[20] , >240 ^[18] , – (sublimation occurs above mpt. @ 99.9 °C, DSC @ 5 K/min, pierced Al pan) ^[18] , 251.2 (exo peak max, DSC @ 5 K/min, sealed Al pan) ^[18]								
ρ [g cm ⁻³]	1.84 (@ 293 K) ^[2, 11] , 1.84 (gas pycnometry) ^[12] , 1.89 ^[13] , 1.554 (@ 105 °C) ^[16] , 1.522 (@ 120 °C) ^[16] , 1.84 ^[18, 24, 30] , 1.86 ^[30] , 1.840 (TMD) ^[33] Measured above mpt. using pycnometry ^[23] : <table><tr><td>T (°C)</td><td>ρ (g cm⁻³)</td></tr><tr><td>105</td><td>1.554</td></tr><tr><td>120</td><td>1.522</td></tr></table>			T (°C)	ρ (g cm ⁻³)	105	1.554	120	1.522
T (°C)	ρ (g cm ⁻³)								
105	1.554								
120	1.522								
Heat of formation	2.81 kcal mol ⁻¹ (ΔH_f , exptl.) ^[14] , 8.7 kcal mol ⁻¹ (ΔH_f) ^[14] , 189.50 kJ/kg (enthalpy of form.) ^[3, 11] , 280 kJ/kg ^[18] , 8.70 kcal/mol (ΔH_f (s)) ^[24] , 189.5 kJ/kg (ΔH_f , ICT thermochemical database) ^[25] , 30.7 kcal/mol (enthalpy of form.) ^[30] , 8.7 kcal/mol (enthalpy of form.) ^[30] , 2.81 kcal/mol (enthalpy of form.) ^[30] , 36.4 kJ/mol (enthalpy of form., exptl.) ^[37] , 62.2 kJ/mol (enthalpy of form., calcd., emp.) ^[37] , –97 kJ/mol (enthalpy of form., calcd., S-D method) ^[37]								
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.						

$-\Delta_{\text{ex}}U^{\circ}$ [kJ kg ⁻¹]	6,229	6,110 ^[10] 5,733 (calcd. LOTUSES) ^[13] 1.63 kcal/g (Q_{max} , calcd.) ^[24] 6,343 (calcd., ICT-code) ^[25] 1,900 (heat of explosion) ^[18] 1,731 cal/g (enthalpy of explosion) ^[30] $-\Delta H_{\text{det.}}$ (calcd. from products @ 298 K, [H ₂ O (l)]) = 6,364 J/g ^[14]	6,343 [H ₂ O (l)] ^[11] 6,024 [H ₂ O (g)] ^[11] $-\Delta H_{\text{det.}}$ (exptl.) = 6,130 J/g (TNAZ purity ≥ 99.8%, detonation calorimetry) ^[14]
T_{ex} [K]	4,115	4,263 (calcd., ICT-code) ^[25] 4,659 ^[30] 4,224 (@ 1.832 g cm ⁻³ , ΔH_f = 11.8 kJ/ mol, calcd., JAGUAR) ^[32]	
$p_{\text{C-J}}$ [kbar]	365	390 ^[10] 34.25 GPa (calcd. LOTUSES) ^[13] 364 (@ 1.84 g cm ⁻³ , calcd.) ^[24] 151–5 MPa (calcd., ICT-code) ^[25] 35.68 GPa ^[30] 35.1 GPa (@ 1.832 g cm ⁻³ , ΔH_f = 11.8 kJ/mol, calcd., JAGUAR) ^[32]	343 ^[8] 33.5 GPa (@ 1.84 g cm ⁻³) ^[22]
VoD [m s ⁻¹]	8,947	8,860 (@ 1.841 g cm ⁻³) ^[10] 8,860 (@ 1.76 g cm ⁻³) (calcd. LOTUSES) ^[13] 8,730 (@ 1.83 g cm ⁻³) ^[19] 9,056 (@ 1.83 g cm ⁻³ , calcd., BKWR) ^[19] 8,977 (@ 1.83 g cm ⁻³ , calcd., BKWS) ^[19] 9,000 (@ 1.84 g cm ⁻³ , calcd.) ^[24] 8,730 (@ 1.832 g cm ⁻³ , ΔH_f = 11.8 kJ/mol, calcd., JAGUAR) ^[32]	8,680 (@ 1.76 g cm ⁻³) ^[8] 8,730 (@ 1.84 g cm ⁻³) ^[22] 8,620 (@ 1.84 g cm ⁻³) ^[22]

V_0 [L kg ⁻¹]	729																																																													
Critical T [°C]	Far above its mpt. ^[33]																																																													
Thermal stability	<p>Moles of gas produced per mole TNAZ/no. of h^[20]:</p> <p>@ 120 °C: 0/22, 0/72^[20]</p> <p>@ 220 °C: 3.01/22, 3/72^[20]</p> <p>@ 320 °C: 3.46/22, 3.77/72^[20]</p> <p>% conversion (η) of TNAZ in <i>m</i>-DNB (% conc. of TNAZ in <i>m</i>-DNB) and in gas-phase over time (min), approx. values from graph^[35]:</p> <table><tr><th>Time (min)</th><th>TNAZ in (g)</th><th>5%</th><th>60%</th><th>80%</th><th>100% (molten TNAZ)</th></tr><tr><td>50</td><td>20</td><td>25</td><td>35</td><td>35</td><td>65</td></tr><tr><td>100</td><td>35</td><td>43</td><td>70</td><td>65</td><td>93</td></tr><tr><td>150</td><td>45</td><td>60</td><td>90</td><td>85</td><td>98</td></tr></table> <p>% conversion (η) of TNAZ in melt over time (min), approx. values from graph^[35]:</p> <table><tr><th>Time (min)</th><th>@ 170 °C</th><th>@ 180 °C</th><th>@ 190 °C</th><th>@ 210 °C</th></tr><tr><td>5</td><td>–</td><td>–</td><td>–</td><td>60</td></tr><tr><td>100</td><td>5</td><td>10</td><td>40</td><td>–</td></tr><tr><td>200</td><td>10</td><td>20</td><td>95</td><td>–</td></tr><tr><td>300</td><td>15</td><td>40</td><td>100</td><td>–</td></tr><tr><td>400</td><td>18</td><td>60</td><td>–</td><td>–</td></tr><tr><td>500</td><td>22</td><td>85</td><td>–</td><td>–</td></tr></table>			Time (min)	TNAZ in (g)	5%	60%	80%	100% (molten TNAZ)	50	20	25	35	35	65	100	35	43	70	65	93	150	45	60	90	85	98	Time (min)	@ 170 °C	@ 180 °C	@ 190 °C	@ 210 °C	5	–	–	–	60	100	5	10	40	–	200	10	20	95	–	300	15	40	100	–	400	18	60	–	–	500	22	85	–	–
Time (min)	TNAZ in (g)	5%	60%	80%	100% (molten TNAZ)																																																									
50	20	25	35	35	65																																																									
100	35	43	70	65	93																																																									
150	45	60	90	85	98																																																									
Time (min)	@ 170 °C	@ 180 °C	@ 190 °C	@ 210 °C																																																										
5	–	–	–	60																																																										
100	5	10	40	–																																																										
200	10	20	95	–																																																										
300	15	40	100	–																																																										
400	18	60	–	–																																																										
500	22	85	–	–																																																										
Vacuum stability test [cm ³ /h]	0.95 mL gas evolved after 48 h @ 100 °C ^[12] , 0.01 cm ³ @ 110 °C, 20 h, $\rho_{\text{(TNAZ)}} = 1.84 \text{ g cm}^{-3}$ ^[23, 26, 28]																																																													
Volatility	Highly volatile and is partially evaporated in a closed system ^[35]																																																													
Solubility [g/mL]	g (TNAZ)/mL (solvent) ^[30] : 0.436 in ethyl acetate, 0.055 in EtOH, 0.026 in isopropanol, 0.442 in acetone, 0.038 in toluene, 0.014 in <i>iso</i> -octane ^[30]																																																													
Hygroscopicity	Nonhygroscopic ^[31]																																																													

Compatibility	Compatibility investigated using vacuum test, 110 °C, 20 h ^[26] : RDX/TNAZ (60/40), $\rho = 1.78$, vol. of gas = 0.10 cm ³ ^[26] , HMX/TNAZ (60/40), $\rho = 1.85$, vol. of gas = 0.04 cm ³ ^[26] , TNAZ/Hyt/DOA (98/1/1), vol. of gas = 0.03 cm ³ ^[26] , HNIW/TNAZ (60/40), $\rho = 1.92$, vol. of gas = 0.25 cm ³ ^[28] , NTO/TNAZ (60/40), $\rho = 1.86$, vol. of gas = 0.02 cm ³ ^[28] , addition of 3 wt. % PA into the melt increases TNAZ dec. by 4 times ^[29] , addition of 0.6 wt. % hexamethylene tetramine into the melt increases TNAZ dec. by 50 times ^[29] , compatible with Al, steel, brass and glass ^[31] , 3% picric acid accelerates TNAZ dec. four-fold ^[35] , 0.6% hexamethylene accelerates TNAZ dec. 50-fold ^[35]					
Detonation calorimetry	96% energy of HMX ^[26] , 150% energy of TNT ^[26]					
ARC (accelerating rate calorimetry)	Adiabatic self-heating only @ ~ 180 °C ^[18]					
Decomposition activation energy [kcal/mol]	46.6 (@ 160–280 °C, closed vessel, 0.2–0.3 mg sample) ^[29] , 40.3 (in soln., 1% in benzene) ^[29] , 133 kJ/mol (DSC) ^[29] , 161.3 kJ/mol (Ozawa method) ^[29] , 157.5 kJ/mol (DTA) ^[29]					
Enthalpy of sublimation [kJ/mol]	95 ^[30] , 63.22 ^[30]					
Enthalpy of vaporization [kJ/mol]	66 ^[30]					
Enthalpy of fusion [kcal/mol]	6.714 ± 0.115 ^[30] , 6.7–7.2 ^[30]					
pK _a	–15.72 ± 0.20 (pH 1–10, calcd.) ^[30]					
K _{oc}	33.7 (pH 1–10, calcd.) ^[30]					
Biodegradation	Half-life in soil is <24 h for several soil types ^[30]					
Slow and fast cook-off test	Detonation @ 198–214 ^[16]					
Wedge test	TNAZ wedges neat-pressed @ 420,000 psi @ 97 °C to final wedge shape, @ 99.1–99.4% TMD (TMD = 1.840 g cm ^{–3}) ^[33] :					
	ρ_0 (g/cm ³)	P_0 (GPa)	u_p (km/s)	U_s (km/s)	x^* (mm)	t^* (μs)
	1.825	2.9	0.47	3.42	8.18	2.36
	1.826	3.9	0.57	3.80	3.73	1.08
	18.26	5.0	0.70	3.95	2.80	0.69
	1.828	7.6	0.93		1.06	0.34

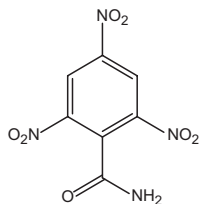
	TNAZ-I ^[17]	TNAZ-II ^[18]
	Stable, higher ρ	Unstable, lower ρ
Chemical formula	$C_3H_4N_4O_6$	$C_3H_4N_4O_6$
Molecular weight [g mol ⁻¹]	192.06	192.06
Crystal system	Orthorhombic	
Space group	$P b c a$ (no. 61)	
a [Å]	5.733(1)	
b [Å]	11.127(2)	
c [Å]	21.496(4)	
α [°]	90	
β [°]	90	
γ [°]	90	
V [Å ³]	1,371.3(3)	
Z	8	
ρ_{calc} [g cm ⁻³]	1.861 ($\rho = 1.84$ g cm ⁻³ @ 20 °C)	
T [K]	-30 °C	
	Recryst. from CCl ₄	

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2,4,6-Trinitrobenzamide

Name [German, acronym]: 2,4,6-Trinitrobenzamide, trinitrobenzamide
 Main (potential) use: explosive
 Structural formula:



	Trinitrobenzamide		
Formula	C ₇ H ₄ N ₄ O ₇		
Molecular mass [g mol ⁻¹]	256.13		
Appearance at RT	yellow crystals from acetone/petroleum ether/benzene ^[2]		
IS [J]	62.8 cm (5 kg mass, AFATL) ^[3]		
N [%]	21.87		
Ω(CO ₂) [%]	−56.22		
T _{m,p.} [°C]	264 (dec.) ^[2]		
T _{dec.} [°C]			
ρ [g cm ⁻³]			
Heat of formation			
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
−Δ _{ex} U° [kJ kg ⁻¹]			
T _{ex} [K]			
p _{C-J} [kbar]			
VoD [m s ⁻¹]			
V ₀ [L kg ⁻¹]			
Dipole moment [D]	2.52 (calcd.) ^[3]		

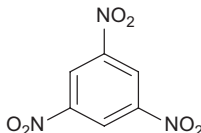
	2,4,6-Trinitrobenzamide^[1]
Chemical formula	C ₇ H ₄ N ₄ O ₇
Molecular weight [g mol ⁻¹]	256.13
Crystal system	Orthorhombic
Space group	<i>Pbca</i> (no. 61)
<i>a</i> [Å]	9.248(3)
<i>b</i> [Å]	14.377(6)
<i>c</i> [Å]	17.729(4)
α [°]	90
β [°]	90
γ [°]	90
<i>V</i> [Å ³]	1,958(1)
<i>Z</i>	8
ρ_{calc} [g cm ⁻³]	1.737
<i>T</i> [K]	295

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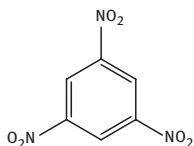
Trinitrobenzene

Name [German, acronym]: 1,3,5-Trinitrobenzene, 2,4,6-trinitrobenzene, sym-trinitrobenzene [trinitrobenzol, TNB, sym-TNB]
 Main (potential) use: Stable secondary explosive with good performance but economically not viable^[15], used in naval Ap shells in World War I^[50]

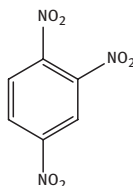
Structural formula:*



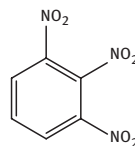
* 3 isomers of TNB are known, most values given are for 1,3,5-TNB (in addition, 1,3,5-TNB exists in two isomorphous forms)^[34]:



1,3,5-Trinitrobenzene
(sym-trinitrobenzene)



1,2,4-Trinitrobenzene



1,2,3-Trinitrobenzene

	TNB
Formula	$C_6H_3N_3O_6$
Molecular mass [g mol ⁻¹]	213.11
Appearance at RT	1,3,5-TNB: pale yellow crystals ^[34] , greenish-yellow leaflet crystals ^[35] , yellow cryst. solid ^[38] , 1,2,4-TNB: pale yellow crystals ^[34] , 1,2,3-TNB: pale yellow crystals ^[34] , 1,3,5-TNB exists in two isomorphous forms @ RT ^[34] , white platelets ^[50] , recryst. from EtOH as white platelets of rhombic shape ^[53] , orthorhombic bipyramidal plates from glacial acetic acid ^[60]
IS [J]	24.52 ^[4] , 5.90 (first reaction) ^[7] , 24.64 (sound) ^[7] , 5.89 ^[14] , 17.40 ^[14] , 11 in (P.A.) ^[16] , FI = 109% PA ^[16] , $H_{50\%} = 100$ cm ^[19, 32] , $H_{50} = 100$ cm ^[20] , 5.70 (Julius-Peters app.) ^[21] , 0.75 kp/m ^[22] , $H_{50\%} = 100$ cm ^[22] , 24.64 (Bruceton method) ^[30, 51] , 50% explosions require impact energy of 12.1 kg/cm ² ^[34] , less impact sensitive than TNT ^[35] , $H_{50\%} = 150$ cm (5 kg mass, contained in small iron 0.2 mm thick cap covered with

	small iron disc) ^[35] , 100 cm (50% initiation height) ^[37, 38] , 103 cm ^[38] , $H_{50} = 71$ cm (17 J) ^[39] , 100 cm (Bruceton method, type 12 tool, 2.5 kg mass, 40 mg sample, 5/0 sandpaper, 25 trials) ^[40] , 100 cm (2.5 kg mass) ^[43] , 49.8 cm (2.5 kg mass, AFATL) ^[43] , $H_{50} = 71$ cm (2.5 kg mass, type 12 tool) ^[46] , $\log(H_{50}) = 2.000$ (Kamlet/Adolph) ^[47] , 1,610 mm (dropheight, Rotter impact test) ^[49] , 986 mm (dropheight, Rotter impact test +5% DETA) ^[49] , 46 cm (2 kg mass) ^[53] , $A_{d1} = 24\%$, $A_{d2} = 4\%$, $A_{50\ d1} = 4.0$ m, $A_{50\ d2} = 7.0$ ^[58] , $H_{50\%} = 71$ cm (2.5 kg mass) ^[62]																
FS [N]	353 ^[15] , $P_{fr,LL} = 650$ MPa ^[18, 58] , $P_{fr,50\%} = 900$ MPa ^[18, 58]																
ESD [J]	6.31 ^[4-6, 14, 63] , 108.2 mJ ^[5]																
N [%]	19.72																
$\Omega(\text{CO}_2)$ [%]	-56.30																
$T_{m.p.}$ [°C]	121-122 ^[1, 35] , 121-122.5 (stable form) ^[16] , 61 (unstable form) ^[16] , 120-122 (commercial TNB, mainly sym-TNB) ^[16] , 121 ^[23, 37, 38] , 121.3 ^[23, 42] , 122.5 ^[31, 60] , 122 (1,3,5-TNB) ^[34] , 62 (1,2,4-TNB) ^[34] , 127.5 (1,2,3-TNB) ^[34] , 122.5 (1,3,5-TNB, isomorph 1) ^[34] , 106.3 (1,3,5-TNB, isomorph-2) ^[34] , 121 (Thomas Hoover Capillary Melting Point Apparatus @ 2 °C/min) ^[42] , 122 ^[48] , 123-125 (freezing point) ^[53]																
$T_{b.p.}$ [°C]	315 ^[31] , 350 ^[33, 51] , 175 (@ 2 mm Hg) ^[36] , 250 (@ 50 mm Hg) ^[36] , 315 ± 10 (@ 760 mm Hg) ^[36]																
$T_{dec.}$ [K]	580 (DTA) ^[7, 21]																
ρ [g cm ⁻³]	1.69-1.73 (@ 293 K) ^[2] , 1.76 ^[15, 32] , 1.688 (@ 20 °C) ^[16] , ρ of compressed pellets ^[35] : <table><tr><td>Pressure (kg/cm²)</td><td>ρ (g/cm³)</td><td>Pressure (kg/cm²)</td><td>ρ (g/cm³)</td></tr><tr><td>275</td><td>1.343</td><td>2,060</td><td>1.641</td></tr><tr><td>685</td><td>1.523</td><td>2,750</td><td>1.654</td></tr><tr><td>1375</td><td>1.620</td><td>3,435</td><td>1.662</td></tr></table> 1.668 (crystal) ^[38] , 1.64 (exptl.) ^[37, 38] , 1.69 (100.0% TMD, pressed, @ loading pressure of 64,000 psi) ^[37] , 1.688 (TMD) ^[37] , 1.63 ^[48] , sp. gr. = 1.69 ^[53] , ρ practically attainable by pressing = 1.65 ^[53] , 1.68 ^[59] , $d_{4}^{20} = 1.76$ ^[60] , $d_{4}^{152} = 1.4775$ ^[60]	Pressure (kg/cm ²)	ρ (g/cm ³)	Pressure (kg/cm ²)	ρ (g/cm ³)	275	1.343	2,060	1.641	685	1.523	2,750	1.654	1375	1.620	3,435	1.662
Pressure (kg/cm ²)	ρ (g/cm ³)	Pressure (kg/cm ²)	ρ (g/cm ³)														
275	1.343	2,060	1.641														
685	1.523	2,750	1.654														
1375	1.620	3,435	1.662														
Heat of formation	-37.2 kJ/mol ($\Delta_f H^\circ$ (s)) ^[10] , -204.2 kJ/kg ($\Delta_f H^\circ$ (s), ICT thermochemical code) ^[3] , -9.0 kcal/mol ^[13] , -8.9 kcal/mol ($\Delta_f H^\circ$ (s)) ^[32] , 21.1 kcal/mol (1,3,5-TNB) ^[34] , 25.8 kcal/mol (1,3,5-TNB) ^[34] , 23.0 kcal/mol (1,3,5-TNB) ^[34] , 10.8 kcal/mol (1,2,4-TNB) ^[34] , -11.40 (exo) kcal/mol (135-TNB) ^[37, 38] , 23.5 kcal/kg ^[52] , -42.0 kcal/kg (enthalpy of form.) ^[41] , -37.2 kJ/mol (ΔH_f) ^[59]																
Heat of combustion	665.6 kcal/mol (Q_c) ^[16] , 3,096 cal/g (Q_c^V) ^[16] , 3,099 kcal/kg (@ C^V) ^[52] , 665.6 kcal/mol (1,3,5-TNB) ^[34] , 667.1 kcal/mol (1,3,5-TNB) ^[34] , 675.9 kcal/mol (1,2,4-TNB) ^[34]																

	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{\text{ex}} U^{\circ}$ [kJ kg ⁻¹]	4,701	<p>5,682 (calcd., K-J)^[10]</p> <p>2,937 (calcd., K-W)^[10]</p> <p>3,862 (calcd. mod. K-W)^[10]</p> <p>$Q_{\text{real}} = 4,540 \text{ MJ kg}^{-1}$^[30]</p> <p>1.36 kcal/g (Q_{max}, calcd.)^[32]</p> <p>1,065 kcal/kg (@ 1.63 g cm⁻³)^[34]</p> <p>766 cal/g (@ 1.640 g cm⁻³, 92.7% TMD)^[37]</p> <p>937 cal/g (calcd. based on heat of formation of TNB and detonation products)^[38]</p> <p>937 cal/g (@ 1.6 g cm⁻³, calcd., Halford– Kistiakowsky– Wilson equation of state)^[38]</p> <p>3,963 (calcd., ICT-code)^[3]</p> <p>1,071 kcal/kg (@ 1.660 g cm⁻³, calcd.) [H₂O vapor]^[41]</p> <p>4,540 MJ•kg⁻¹ (Q_{real}, calcd., semi- empirical Pepekina method)^[51]</p> <p>5.34 MJ/kg (heat of explosion)^[54]</p> <p>$-\Delta H_{\text{det}} = 5.85 \text{ kJ/g}$^[59]</p>	<p>3,964 [H₂O (l)]^[9, 15]</p> <p>3,876 cal/kg [H₂O (g)]^[13]</p> <p>1,100 cal/kg [H₂O (g)]^[13]</p> <p>1,063 cal/g^[16]</p> <p>811 cal/g (Q, det. energy from aquarium measurements)^[38]</p> <p>1,100 kcal/kg (@ 1.660 g cm⁻³) [H₂O vapor]^[41]</p> <p>1,104 kcal/kg^[53]</p>

T_{ex} [K]	3,524	3,540 °C (@ 1.63 g cm ⁻³) ^[34] 2,950 (@ 1.6 g cm ⁻³ , calcd., Halford– Kistiakowsky– Wilson equation of state) ^[38] 3,017 (calcd., ICT-code) ^[3]	3,549 (max.) ^[16]
$p_{\text{C-J}}$ [kbar]	220	215 (@ 1.64 g cm ⁻³ , calcd., K-J) ^[10] 228 (@ 1.64 g cm ⁻³ , calcd., K-W) ^[10] 228 (@ 1.64 g cm ⁻³ , calcd., mod. K-W) ^[10] 248 (@ 1.76 g cm ⁻³ , calcd.) ^[32] 214 (@ 1.640 g cm ⁻³ , 92.7% TMD) ^[37] 181.4 (@ 1.6 g cm ⁻³ , calcd., Halford– Kistiakowsky– Wilson equation of state) ^[38] 119.6 MPa (calcd., ICT- code) ^[3]	219 ^[10, 27] 219.2 ^[24]
VoD [m s ⁻¹]	7,304 (@ 1.71)	7,170 (@ 1.64 g cm ⁻³ , calcd., K-J) ^[10] 7,380 (@ 1.64 g cm ⁻³ , calcd., K-W) ^[10] 7,390 (@ 1.64 g cm ⁻³ , calcd., mod. K-W) ^[10] 6,970 (@ 1.65 g cm ⁻³ , calcd., K-J) ^[25] 7,160 (@ TMD) ^[27] 7,400 (@ 1.65 g cm ⁻³ , average value from lit.) ^[16]	7,330 (@ 1.71 g cm ⁻³) ^[15] 7,270 (@ 1.64 g cm ⁻³) ^[8, 10] 7,450 (@ 1.60 g cm ⁻³) ^[12] 7,000 (@ 1.64 g cm ⁻³) ^[16] 7,350 (@ 1.60 g cm ⁻³ , in 20 mm diameter paper cartridge) ^[16] 7,350 (@ 1.66 g cm ⁻³) ^[16]

		7,270 (@ TMD, calcd. R-P method) ^[26] 7,510 (@ TMD, calcd., K-J) ^[30] 7,530 (@ 1.76 g cm ⁻³ , calcd.) ^[32] 3,990 (@ 0.7 g cm ⁻³) ^[34] 7,269 (@ 1.640 g cm ⁻³ , 92.7% TMD) ^[37, 38] 7,082 (@ 1.6 g cm ⁻³ , calcd., Halford–Kistiakowsky–Wilson equation of state) ^[38]	7,440 (@ 1.68 g cm ⁻³ , cast explosive) ^[16] 7,441 (cast TNB, measured as function of charge ρ , Dautriche method) ^[35, 38] 7,270 (@ TMD) ^[27] 7,287 (calcd. based on sand test) ^[16] 7,269 (@ 1.644 g cm ⁻³) ^[24] 7,150 (@ 1.65 g cm ⁻³) ^[22] 7,300 (@ 1.71 g cm ⁻³) ^[30, 51] 7,347 (column of 10 pellets, 20 mm diameter weighing 8 g each, @ 1.641 or 1.662 g cm ⁻³ , paper cartridge, initiator = MF and 80 g dynamite, Dautriche) ^[35] <i>see extra table at end of section</i>
V_0 [L kg ⁻¹]	637	670 (@ 1.63 g cm ⁻³) ^[34] 0.4837 cm ³ /g (@ 1.6 g cm ⁻³ , calcd., Halford–Kistiakowsky–Wilson equation of state) ^[38]	805 ^[11, 15] 711 ^[53]

Critical diameter [cm]	Data from ^[56] :		
	ρ_0 (g/cc)	% TMD	d_c (cm)
	1.64	97.2 \pm 0.3	\leq 0.3
Trauzl test [cm ³ , % TNT]	111% TNT ^[16] , 108% PA ^[16] , 330 cc ^[28, 34] , 108–111% PA ^[34] , 325 cc/10 g ^[22] , 105–120% TNT ^[16] , 480 cc (15 g TNB) ^[35] , 325 ^[57] , 386 ^[57]		
Sand test [g]	110% TNT ^[16] , 43.2 g sand crushed (1,700 g bomb, 0.4 g TNB) ^[16]		

Ballistic mortar test	105–117% TNT ^[16] , more powerful, more brisant than TNT ^[35]																																																						
SSGT [cm]	<p>P_{90} = 14.96 kbar (P_{90} = pressure to 90% of TMD, NSW small-scale gap test)^[40]</p> <p>TNB TMD = 1.69, (1) = no mixed response zone, (2) = experimental error, data from^[45]:</p> <table><tr><th rowspan="2">Loading pressure (kpsi)</th><th colspan="2">Density (g/cm³)</th><th rowspan="2">% TMD</th><th colspan="4">Sensitivity (DBG)</th></tr><tr><th>AVG.</th><th><i>s</i></th><th>AVG.</th><th><i>g</i></th><th><i>s_m</i></th><th><i>N</i></th></tr><tr><td>4</td><td>1.239</td><td>0.007</td><td>73.3</td><td>3.587</td><td>–</td><td>–</td><td>19 (1)</td></tr><tr><td>8</td><td>1.390</td><td>0.008</td><td>82.2</td><td>3.848</td><td>0.2588</td><td>0.1648</td><td>20</td></tr><tr><td>16</td><td>1.547</td><td>0.005</td><td>91.5</td><td>5.118</td><td>0.0094</td><td>0.0075</td><td>20</td></tr><tr><td>32</td><td>1.647</td><td>0.003</td><td>97.5</td><td>6.102</td><td>0.0888</td><td>0.0502</td><td>20</td></tr><tr><td>64</td><td>1.692 (2)</td><td>0.003</td><td>100.1</td><td>8.646</td><td>0.1600</td><td>0.0925</td><td>29</td></tr></table>	Loading pressure (kpsi)	Density (g/cm ³)		% TMD	Sensitivity (DBG)				AVG.	<i>s</i>	AVG.	<i>g</i>	<i>s_m</i>	<i>N</i>	4	1.239	0.007	73.3	3.587	–	–	19 (1)	8	1.390	0.008	82.2	3.848	0.2588	0.1648	20	16	1.547	0.005	91.5	5.118	0.0094	0.0075	20	32	1.647	0.003	97.5	6.102	0.0888	0.0502	20	64	1.692 (2)	0.003	100.1	8.646	0.1600	0.0925	29
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Small-scale gap (booster) sensitivity test	<p>Pressed TNB, values from^[37], $DB_g = 30 - 10 \log (\text{test gap}/\text{ref. gap})$^[37]:</p> <table><tr><th colspan="2">@ 93% TMD</th><th colspan="2">@ 95% TMD</th></tr><tr><td>DBG</td><td>Lucite gap (mils)</td><td>DBG</td><td>Lucite gap (mils)</td></tr><tr><td>5.2</td><td>303</td><td>5.7</td><td>269</td></tr></table>	@ 93% TMD		@ 95% TMD		DBG	Lucite gap (mils)	DBG	Lucite gap (mils)	5.2	303	5.7	269																																										
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5 s explosion <i>T</i> [°C] Explosion <i>T</i> [°C] 5 s ignition <i>T</i> [°C] Ignition <i>T</i> [°C]	520 ^[16, 38] 550 ^[24, 44] 347 (calcd. based on exptl. bpt.) ^[30, 51] , 363 (calorimetric measured) ^[44]																																																						
Thermal stability [°C]	283 (threshold of thermal stability) ^[51] , can be sublimed on careful heating but explodes if rapidly heated ^[60]																																																						
Vacuum stability test [cm ³ /h]	0.046 cc/5 g in 48 h @ 120 °C ^[16] , <0.10 cc/g/h (average for 2 h exposure) @ 260 °C ^[37] , 0.0 cm ³ /g/48 h @ 100 °C ^[38] , <0.10 cm ³ /g/h @ 260 °C (2 h exposure) ^[38]																																																						
Vapor pressure [atm. @ °C]	2.2×10^{-14} Torr @ 20 °C ^[31] , 3.03×10^{-6} Torr @ 25 °C ^[48]																																																						

Solubility [g/mL]

34 mg/L H₂O @ 20 °C^[31], moderately soluble in hot EtOH^[35], more soluble in acetone, Et₂O, benzene^[35], aqueous solubility = ~ 385 mg/L @ 25 °C^[48]

Solubility (g) of *sym*-TNB in 100 g solvent^[34]:

Solvent	T (°C)		
	17	50	100
MeOH	3.76	7.62	–
EtOH	2.09	4.57	–
Et ₂ O	1.70	2.72 (@ 32 °C)	–
Acetone	59.11	160.67	–
CS ₂	0.24	0.44 (@ 33 °C)	–
CHCl ₃	6.24	18.42	–
Benzene	6.18	25.70	–
Toluene	11.86	46.31	–
Pyridine	112.60	194.23	–
Ethyl acetate	29.83	52.40	–
H ₂ O	0.03	0.10	0.50

Best solvents for TNB are pyridine and acetone^[53]

Solubility of TNB (g) in 100 g solvent @ T (°C)^[53]:

Solvent	Solubility of TNB (g) in 100 g solvent		
	17 °C	50 °C	100 °C
Pyridine	112.60	194.23	–
Acetone	59.11	160.67	–
Ethylacetate	29.83	52.40	–
Toluene	11.86	46.31	–
Benzene	6.18	25.70	–
Chloroform	6.24	18.42	–
Methanol	3.76	7.62	–
Ethanol	2.09	4.57	–
Ether	1.70	2.72 @ 32 °C	–
Carbon disulfide	0.24	0.44 @ 33 °C	–
Water	0.03	0.10	0.50

	Solubility of TNB in sulfuric acid ^[53] :																																																					
	<table><tr><th rowspan="2">T(°C)</th><th colspan="4">% Solubility of TNB in sulfuric acid (strength in %)</th></tr><tr><th>70%</th><th>80%</th><th>90%</th><th>100%</th></tr><tr><td>25</td><td>0.5</td><td>1.05</td><td>7.8</td><td>21.5</td></tr><tr><td>40</td><td>0.75</td><td>1.75</td><td>8.6</td><td>24.0</td></tr><tr><td>50</td><td>0.9</td><td>1.9</td><td>11.3</td><td>26.5</td></tr><tr><td>60</td><td>1.15</td><td>2.3</td><td>11.65</td><td>28.0</td></tr><tr><td>70</td><td>1.2</td><td>2.95</td><td>12.05</td><td>32.0</td></tr><tr><td>80</td><td>1.5</td><td>3.75</td><td>14.75</td><td>34.3</td></tr><tr><td>90</td><td>2.0</td><td>4.15</td><td>17.75</td><td>37.0</td></tr><tr><td>100</td><td>25</td><td>5.90</td><td>21.30</td><td>42.4</td></tr></table>					T(°C)	% Solubility of TNB in sulfuric acid (strength in %)				70%	80%	90%	100%	25	0.5	1.05	7.8	21.5	40	0.75	1.75	8.6	24.0	50	0.9	1.9	11.3	26.5	60	1.15	2.3	11.65	28.0	70	1.2	2.95	12.05	32.0	80	1.5	3.75	14.75	34.3	90	2.0	4.15	17.75	37.0	100	25	5.90	21.30	42.4
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	Solubility (g/100 g solvent): 0.035 in H ₂ O ^[60] , 6.2 in benzene ^[60] , 4.9 in MeOH ^[60] , 1.9 in EtOH ^[60] , 1.5 in Et ₂ O ^[60] , 0.25 in CS ₂ ^[60] , 0.05 in petrol ether ^[60] , freely soluble in dilute Na ₂ SO ₃ soln. ^[60]																																																					
Compatibility	Does not react with metals or oxides thereof ^[53] , reacts with alcoholic solns. of bases ^[53] , reduction by Sn in hydrochloric acid occurs ^[53] , transformed by certain oxidizers to PA ^[53] , reacts with gaseous NH ₃ @ LT ^[53]																																																					
Dipole moment [D]	0.26 (calcd.) ^[43] , 0.00 (exptl.) ^[43]																																																					
Plate push value	2,946 ft/s @ 98% TMD (calcd. from measurements at other ρ) ^[37] , 2,841 ft/s @ 93% TMD (calcd. from measurements at other ρ) ^[37] , failure diameter <0.3 cm ^[37]																																																					
Wedge test	3–10 mm thick TNB pellets of $\rho = 1.69 \text{ g cm}^{-3}$, shocked to ~90 kb, an initial instantaneous shock wave velocity of 6,800 m/s was obtained, values from ^[38] : <table><tr><td>Brass thickness (cm)</td><td>Initial shock velocity H.E. (m/s)</td><td>Initial particle velocity H.E. (m/s)</td><td>Initial shock pressure H.E. (V, V₀)</td><td>ρ_0 H.E. (g/cm³)</td><td>D (final) (m/s)</td></tr><tr><td>1.27</td><td colspan="3">(Only reactive shock was observed)</td><td>1.372</td><td>6,400</td></tr></table>					Brass thickness (cm)	Initial shock velocity H.E. (m/s)	Initial particle velocity H.E. (m/s)	Initial shock pressure H.E. (V, V ₀)	ρ_0 H.E. (g/cm ³)	D (final) (m/s)	1.27	(Only reactive shock was observed)			1.372	6,400																																					
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1.27	(Only reactive shock was observed)			1.372	6,400																																																	
ΔH_{sub} [kJ/mol]	107.3 (exptl.) ^[45] , 99.2 (calcd., QSPR) ^[45]																																																					
Diffusion coefficient [cm ² /s]	0.68 (air) ^[48] , 7.20×10^{-6} (water) ^[48]																																																					
Heat of fusion [cal/g]	16.0 ^[48]																																																					

Log K_{ow}	1.18 ^[48]																																																				
Log K_{oc}	1.30 ^[48]																																																				
Biodegradation	TNB found to persist in soils and wastewater lagoon sediments years after a production facility became redundant ^[48] , under certain conditions TNB found to be not biodegradable ^[48]																																																				
Fugacity	325 cc ^[53]																																																				
Brisance (Kast)	4.7 mm ^[53]																																																				
Closed vessel test	Gas pressure (exptl.) by explosions in small bomb, pressure measured by piston and obturator ^[29, 35] ; loading $\rho = 0.20 \text{ g cm}^{-3}$, pressure = 2,205 kg/cm ² ^[29, 35] , loading $\rho = 0.25 \text{ g cm}^{-3}$, pressure = 3,050 kg/cm ² ^[29, 35] , loading $\rho = 0.30 \text{ g cm}^{-3}$, pressure = 4,105 kg/cm ² ^[29, 35] Pressure = 3,925 kg/cm ² (@ 0.3 g cm ⁻³ , manometric bomb) ^[35] Explosion $T = 2,356 \text{ }^{\circ}\text{C}$ (@ 0.3 g cm ⁻³ , manometric bomb) ^[35]																																																				
Radiation sensitivity	<p>Data from^[61]:</p> <table><tr><th rowspan="2">Exposure rate (R/h)</th><th rowspan="2">Total dose (R)</th><th colspan="2">Vacuum stability test</th></tr><tr><th>100 $^{\circ}\text{C}$ (cc/g/40 h)</th><th>200 $^{\circ}\text{C}$ (cc/.2 g/2 h)</th></tr><tr><td rowspan="4">9.2×10^5</td><td>Control</td><td>0.46</td><td>0.08</td></tr><tr><td>1.5×10^7</td><td>0.24</td><td>0.22</td></tr><tr><td>1.3×10^8</td><td></td><td>0.39</td></tr><tr><td>1.0×10^9</td><td>4.10</td><td>1.45</td></tr></table> <p>DTA for irradiated explosives @ 20 $^{\circ}\text{C}/\text{min}$^[61]:</p> <table><tr><th rowspan="3">Total dose (R)</th><th colspan="4">Endotherms</th></tr><tr><th colspan="2">First</th><th colspan="2">Second</th></tr><tr><th>Onset ($^{\circ}\text{C}$)</th><th>Peak ($^{\circ}\text{C}$)</th><th>Onset ($^{\circ}\text{C}$)</th><th>Peak ($^{\circ}\text{C}$)</th></tr><tr><td>0</td><td>110</td><td>121</td><td>325</td><td>352</td></tr><tr><td>1.5×10^7</td><td>100</td><td>119</td><td>337</td><td>347, 351</td></tr><tr><td>1.3×10^8</td><td>100</td><td>120</td><td>325</td><td>356, 361</td></tr><tr><td>1.0×10^9</td><td>90</td><td>112</td><td>300</td><td>345</td></tr></table>	Exposure rate (R/h)	Total dose (R)	Vacuum stability test		100 $^{\circ}\text{C}$ (cc/g/40 h)	200 $^{\circ}\text{C}$ (cc/.2 g/2 h)	9.2×10^5	Control	0.46	0.08	1.5×10^7	0.24	0.22	1.3×10^8		0.39	1.0×10^9	4.10	1.45	Total dose (R)	Endotherms				First		Second		Onset ($^{\circ}\text{C}$)	Peak ($^{\circ}\text{C}$)	Onset ($^{\circ}\text{C}$)	Peak ($^{\circ}\text{C}$)	0	110	121	325	352	1.5×10^7	100	119	337	347, 351	1.3×10^8	100	120	325	356, 361	1.0×10^9	90	112	300	345
Exposure rate (R/h)	Total dose (R)			Vacuum stability test																																																	
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TGA for irradiated explosives^[61]:

Total dose (R)	Heating rate (°C/min)	Weight (mg)	Start of dec (°C)	10% weight loss T (°C)	Total weight loss (%)
0	20	6.2	155	218	97 @ 285 °C
1.5×10^7	20	8.3	155	208	95 @ 265 °C
1.3×10^8	20	8.5	150	209	97 @ 275 °C
1.0×10^9	20	7.4	125	180	97 @ 245 °C
0	10	8.3	130	188	94 @ 245 °C
1.5×10^7	10	8.2	135	192	97 @ 247 °C
1.3×10^8	10	8.75	130	189	99 @ 250 °C
0	50	8.0	175	248	95% @ 325 °C
1.5×10^7	50	8.2	160	236	98 @ 305 °C
1.3×10^8	50	8.1	160	232	96 @ 300 °C
0	80	9.2	195	267	96 @ 355 °C
1.5×10^7	80	8.7	175	251	97 @ 330 °C
1.3×10^8	80	7.9	170	242	95 @ 320 °C

Effect of gamma radiation on the mpt. and color^[61]:

Total dose (R)	mpt. (°C)	Color
0	120	Pale yellow
1.5×10^7	120	Yellow
1.3×10^8	120	Yellow
1.0×10^9	113	Brown

IS for irradiated explosives, 50% fire height in inches, Bruceton method (P.A. apparatus, 2 kg mass)^[61]:

Total Co ⁶⁰ gamma dose (R)	\bar{X} mean (in)	σ std. dev. (in)
0	23.26	4.58
1.5×10^7	18.5	2.96
1.3×10^8	20.5	1.89
1.0×10^9	32.5	4.15

	Effect of gamma radiation on explosion T (5 s explosion T in °C) and activation energy (kcal/mol) ^[61] :				
	Total dose (R)	5 s explosion T (°C)	Apparent activation energy (kcal/mol)		
	0	452	24.86		
	0.5×10^7	434	42.28		
	1.3×10^8	458	19.47		
	Effect of gamma radiation on rates of detonation ^[61] :				
	Total dose (R)	Density (g/cc)	Density after irradiation (g/cc)	Rate of detonation (m/s)	Detonation pressure (kbar)
	0	1.65	–	7,150	211
	1.0×10^7	1.65	1.63	7,115	206
	1.0×10^8	Pellets crumbled			

	TNB ^[2]	TNB ^[2]	TNB ^[2]	TNB ^[17]
Chemical formula	C ₆ H ₃ N ₃ O ₆	C ₆ H ₃ N ₃ O ₆	C ₆ H ₃ N ₃ O ₆	C ₆ H ₃ N ₃ O ₆
Molecular weight [g mol ^{−1}]	213.11	213.11	213.11	213.11
Crystal system	Orthorhombic	Orthorhombic	Monoclinic	Orthorhombic
Space group	<i>P b c a</i> (no. 61)	<i>P c a 2</i> ₁ (no. 29)	<i>P2</i> ₁ / <i>c</i> (no. 14)	<i>P b c a</i> (no. 61)
<i>a</i> [Å]	12.587(11)	9.2970(19)	12.896(5)	9.78(1)
<i>b</i> [Å]	9.684(9)	18.730(4)	5.723(2)	26.94(1)
<i>c</i> [Å]	26.86(2)	9.6330(19)	11.287(5)	12.82(1)
<i>α</i> [°]	90	90	90	90
<i>β</i> [°]	90	90	98.190(8)	90
<i>γ</i> [°]	90	90	90	90
<i>V</i> [Å ³]	3,274(5)	1,677.4(6)	824.5(6)	3,377.73
<i>Z</i>	16	8	4	16

ρ_{calc} [g cm ⁻³]	1.729	1.688	1.717	1.676
T [K]	183	120	183	295
				Neutron diffraction

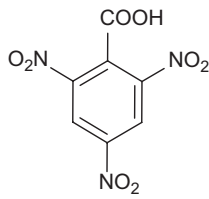
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Trinitrobenzoic acid

Name [German, acronym]: 2,4,6-Trinitrobenzoic acid [trinitrobenzoesäure, TNBA]
Main (potential) use: salts as primary explosives
Structural formula:



	Trinitrobenzoic acid
Formula	C ₇ H ₃ N ₃ O ₈
Molecular mass [g mol ⁻¹]	257.11
Appearance at RT	Orthorhombic crystals from water ^[22]
IS [J]	10 Nm ^[9] , 26.82 ^[4] , 8.28 (first reaction) ^[5, 12, 16] , 26.82 (sound) ^[5, 16] , log H _{50%} = 2.04 ^[8] , comparable to TNT ^[10] , H _{50%} = 109 cm ^[12, 13, 15] , 109 cm (Bruceton method, type 12 tool, 2.5 kg mass, 40 mg sample, 5/0 sandpaper, 25 trials) ^[17] , 109 cm (2.5 kg mass) ^[18] , 91.4 cm (2.5 kg mass, AFATL) ^[18] , H ₅₀ = 109 cm (2.5 kg mass, type 12 tool) ^[19] , log(H ₅₀) = 2.037 (Kamlet/Adolph) ^[20]
FS [N]	353 ^[9]
N [%]	16.34
Ω(CO ₂) [%]	-46.67
T _{m.p.} [°C]	228.7 ^[1, 22] , 228.5–229 (dec.) ^[10]
T _{dec.} [°C]	504 K (DTA onset) ^[16]
ρ [g cm ⁻³]	1.870 (@ 293 K) ^[2] , 1.786 ^[15]
Heat of formation	-409.7 kJ/mol (Δ _f H° (s)) ^[3] , -1,567 kJ/kg (enthalpy of form.) ^[9] , 95.1 kcal/mol (Q _f ^V) ^[10] , -97.9 kcal/mol (Δ _f H (s)) ^[15]
Heat of combustion	-2,773.7 kJ/mol (Δ _c H°) ^[3]

	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^{\circ}$ [kJ kg ⁻¹]	4,110	1.15 kcal/g (Q_{max} , calcd.) ^[15]	667.7 kcal mol ⁻¹ (Q_{e}^{v}) ^[10] 3,008 [H ₂ O (l)] ^[6, 9] 2,929 [H ₂ O (g)] ^[9]
T_{ex} [K]	3,139		
$p_{\text{C-J}}$ [kbar]	241	239 (@ 1.786 g cm ⁻³ , calcd.) ^[15]	
VoD [m s ⁻¹]	7,558 (@ TMD)	7,350 (@ 1.786 g cm ⁻³ , calcd.) ^[15]	
V_0 [L kg ⁻¹]	593		809 ^[7]

Trauzl test [cm ³ , % TNT]	283 cm ³ ^[21]
Ballistic mortar test	98% TNT ^[10]
Thermal stability	Sublimes with dec. ^[22]
Solubility [g/mL]	2.05% w/w in H ₂ O @ 25 ^o ^[22] , 26.6% w/w in EtOH @ 25 ^o ^[22] , 14.7% w/w in Et ₂ O @ 25 ^o ^[22] , soluble in acetone, MeOH ^[22] , slightly soluble in benzene ^[22]
Dipole moment [D]	1.15 (calcd.) ^[18]

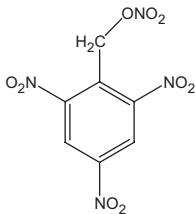
	TNBA ^[14]
Chemical formula	C ₇ H ₃ N ₃ O ₈
Molecular weight [g mol ⁻¹]	257.11
Crystal system	Orthorhombic
Space group	<i>P</i> 2 ₁ 2 ₁ 2 ₁
<i>a</i> [Å]	6.553(1)
<i>b</i> [Å]	11.405(2)
<i>c</i> [Å]	12.796(2)
α [°]	90
β [°]	90

γ [°]	90
V [Å ³]	956.334
Z	4
ρ_{calc} [g cm ⁻³]	1.786
T [K]	295

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2,4,6-Trinitrobenzyl nitrate

Name [German, acronym]: 2,4,6-Trinitrobenzyl nitrate [TNBzIN]
Main (potential) use: high explosive
Structural formula:



	TNBzIN		
Formula	C ₇ H ₄ N ₄ O ₉		
Molecular mass [g mol ⁻¹]	288.13		
Appearance at RT			
IS [J]	Less sensitive than PETN ^[1]		
FS [N]	Less sensitive than RDX ^[1]		
N [%]	19.44		
Ω(CO ₂) [%]	-38.9		
T _{m,p.} [°C]	118.5–119.5 ^[1]		
T _{dec.} [°C]			
ρ [g cm ⁻³]	1.5 (cryst.) ^[1]		
Heat of formation	27.8 kcal/mol (Δ _f H) ^[1]		
Heat of combustion	769.8 kcal/mol (Δ _c H) ^[1]		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
-Δ _{ex} U° [kJ kg ⁻¹]			272.6 kcal/mol ^[1]
T _{ex} [K]			3,885 ^[1]
p _{C-J} [kbar]			
VoD [m s ⁻¹]			
V ₀ [L kg ⁻¹]			

Trauzl test [cm ³ / % TNT]	– /135 ^[1]
Ballistic mortar test [% TNT]	126–127 ^[1]
5 s explosion <i>T</i> [°C] Ignition <i>T</i> [°C]	~340 ^[1]
100 °C heat test [% mass loss]	No explosion in >300 min ^[1]

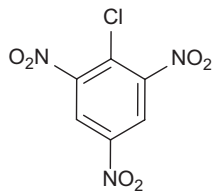
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Trinitrochlorobenzene

Name [German, acronym]: Trinitrochlorobenzene, 1-chloro-2,4,6-trinitrobenzene, picryl chloride [trinitrochlorbenzol, TNCB, CTB]

Main (potential) use: Used as high explosive filler in ammunition in past

Structural formula:



	Picryl chloride
Formula	C ₆ H ₂ N ₃ O ₆ Cl
Molecular mass [g mol ⁻¹]	247.55
Appearance at RT	
IS [J]	16 Nm ^[2] , 11.0 ^[7] , 99% of TNT (2 kg mass) ^[9] , FI = 111–127% PA ^[9] , 79 cm (Bruceton method, type 12 tool, 2.5 kg mass, 40 mg sample, 5/0 sandpaper, 25 trials) ^[15] , 79 cm (2.5 kg mass) ^[16] , 72.5 (5 kg mass AFATL) ^[16]
FS [N]	>353 ^[2]
ESD [J]	6.71 ^[3, 4, 7, 19] , 101.0 mJ ^[3]
N [%]	16.97
Ω(CO ₂) [%]	−45.24
T _{m.p.} [°C]	83 ^[1, 9] , 81.5–83 ^[14]
T _{dec.} [°C]	395–400 (DSC @ 5 °C/min)
ρ [g cm ⁻³]	1.797 (@ 293 K) ^[2, 9] , sp. gr. = 1.76 (molten and then solidified) ^[14]
Heat of formation	108.2 kJ/kg (enthalpy of form.) ^[2] , −36.2 kcal/kg ^[17] , 20.8 kJ/mol (enthalpy of form., exptl.) ^[18] , −51.5 kJ/mol (enthalpy of form., calcd., emp.) ^[18]
Heat of combustion	643 kcal/mol ^[9] , 2,609 kcal/kg (@ C ^v) ^[17]

	Calcd. (EXPLO5 6.03)	Exptl.
$-\Delta_{\text{ex}}U^\circ$ [kJ kg ⁻¹]	4,466	2,845 [H ₂ O (g)] ^[5]
T_{ex} [K]	3,817	3,370 (calcd.) ^[9]
$p_{\text{C-J}}$ [kbar]	233	
VoD [m s ⁻¹]	7,368 (@ 1.74 g/cc)	6,855 (@ 1.70–1.71 g cm ⁻³) ^[9] 7,130 (@ 1.74–1.75 g cm ⁻³) ^[9] 7,347 (@ 1.77 g cm ⁻³) ^[9] 7,200 (@ 1.74 g cm ⁻³) ^[2, 6] 6,450 (@ 1.5 g cm ⁻³) ^[5] 7,130 (@ 1.75 g cm ⁻³) ^[10] 6,930 (@ 1.68 g cm ⁻³) ^[11]
V_0 [L kg ⁻¹]	644	620 ^[9]

Trauzl test [cm ³ , % TNT]	103–110% TNT ^[10] , 97–102% PA ^[9]																															
Solubility [g/mL]	<p>Sparingly soluble in H₂O^[14], 0.0178 parts per 100 parts H₂O @ 15 °C^[14], 0.346 parts per 100 parts H₂O @ 100 °C^[14]</p> <p>Solubility (g) per 100 g solvent^[14]:</p> <table><tr><th>Solvent</th><th>@ 17 °C</th><th>@ 50 °C</th></tr><tr><td>MeOH</td><td>10.24</td><td>34.8</td></tr><tr><td>EtOH (abs.)</td><td>4.48</td><td>15.1</td></tr><tr><td>Et₂O</td><td>7.23</td><td>10.6 (@ 31 °C)</td></tr><tr><td>Ethyl acetate</td><td>91.5</td><td>238.55</td></tr><tr><td>Acetone</td><td>212.0</td><td>546.4</td></tr><tr><td>CHCl₃</td><td>12.36</td><td>233.4</td></tr><tr><td>CCl₄</td><td>0.56</td><td>2.45</td></tr><tr><td>Benzene</td><td>36.39</td><td>428.1</td></tr><tr><td>Toluene</td><td>89.44</td><td>321.1</td></tr></table>		Solvent	@ 17 °C	@ 50 °C	MeOH	10.24	34.8	EtOH (abs.)	4.48	15.1	Et ₂ O	7.23	10.6 (@ 31 °C)	Ethyl acetate	91.5	238.55	Acetone	212.0	546.4	CHCl ₃	12.36	233.4	CCl ₄	0.56	2.45	Benzene	36.39	428.1	Toluene	89.44	321.1
Solvent	@ 17 °C	@ 50 °C																														
MeOH	10.24	34.8																														
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CCl ₄	0.56	2.45																														
Benzene	36.39	428.1																														
Toluene	89.44	321.1																														

Compatibility	Undergoes partial hydrolysis in hot H ₂ O ^[14]
Dipole moment [D]	0.85 (calcd.) ^[16]

	Picryl chloride ^[8]	Picryl chloride ^[12]	Picryl chloride ^[13]
Chemical formula	C ₆ H ₂ N ₃ O ₆ Cl	C ₆ H ₂ N ₃ O ₆ Cl	C ₆ H ₂ N ₃ O ₆ Cl
Molecular weight [g mol ⁻¹]	247.55	247.55	247.55
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	<i>P</i> 2 ₁ / <i>a</i>	<i>P</i> 2 ₁ / <i>a</i>	<i>I</i> 2/ <i>m</i>
<i>a</i> [Å]	11.020(4)	11.10	24.88
<i>b</i> [Å]	6.795(1)	6.83	6.80
<i>c</i> [Å]	14.964(4)	12.62	11.00
α [°]	90	90	90
β [°]	124.15(2)	102.50	102.68
γ [°]	90	90	90
<i>V</i> [Å ³]	927.308	934.081	1,815.64
<i>Z</i>	4	4	8
ρ_{calc} [g cm ⁻³]	1.773	1.76	1.811
<i>T</i> [K]	295	163	295

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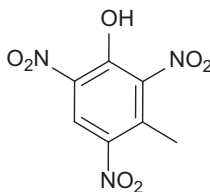
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2,4,6-Trinitrocresol

Name [German, acronym]: 2,4,6-Trinitrocresol, 2,4,6-trinitro-*m*-cresol, 3-Methyl-2,4,6-trinitrophenol, cresylite, 3-methylpicric acid [trinitrometakresol, Kresylit, TNCr]

Main (potential) use: Used as grenade filler in the past^[9], and as a bursting charge in projectiles, ammonium salt has been used in explosive mixtures^[18], not used on its own but used in alloys with PA (e.g. in Cresolite)^[25]

Structural formula:



	2,4,6-Trinitrocresol
Formula	$C_7H_5N_3O_7$
Molecular mass [g mol ⁻¹]	243.13
Appearance at RT	Yellow needles (if recryst. from H ₂ O) ^[18] , bright yellow crystalline substance ^[25]
IS [J]	12 Nm ^[9] , 9.40 (first reaction) ^[4, 19] , 47.00 (sound) ^[4, 19] , slightly more sensitive than PA ^[10] , $H_{50\%} = 191$ cm ^[11] , similar to that of PA ^[17] , $H_{50} = 191$ cm (2.5 kg mass, type 12 tool) ^[21] , $\log(H_{50}) = 2.281$ (Kamlet/Adolph) ^[22]
FS [N]	353 ^[9]
ESD [J]	5.21 ^[3, 27]
<i>N</i> [%]	17.28
$\Omega(\text{CO}_2)$ [%]	-62.52
$T_{\text{m.p.}}$ [°C]	105–108 ^[1] , 106.5–110 ^[10] , 107–107.5 ^[17] , 107 ^[18] , 109 ^[23] , 109.5 ^[25]
$T_{\text{dec.}}$ [°C]	210 (DSC @ 5 °C/min), 468 K (DTA) ^[4] , ~ 200 ^[17] , 488 (DTA) ^[19] , 200 (dec. begins) ^[25]
ρ [g cm ⁻³]	1.740 (@ 293 K) ^[2] , 1.68 ^[8] , 1.69 ^[10] , 1.64 (by pressing and pouring) ^[25]
Heat of formation	252.3 kJ/mol ($\Delta_f H$) ^[5] , -1,038 kJ/kg (enthalpy of form.) ^[9] , 226.7 kcal/kg ^[24] , -54.1 kcal/mol (heat of form., ΔH_f) ^[17] , -248.0 kcal/kg (enthalpy of form.) ^[20]
Heat of combustion	771 cal/mol (C ^V) ^[10] , 3,175 kcal/kg (@ C ^V) ^[24]

	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^\circ$ [kJ kg ⁻¹]	4,117	925 kcal/kg ^[17] 942 kcal/kg (@ 1.580 g cm ⁻³ , calcd.) [H ₂ O vapor] ^[20]	3,370 [H ₂ O (l)] ^[5, 9] 3,248 [H ₂ O (g)] ^[9] 912 kcal/kg [H ₂ O (g)] ^[8] 912 kcal/kg (@ 1.580 g cm ⁻³) [H ₂ O (vapor)] ^[20] 912 kcal/kg ^[25]
T_{ex} [K]	3,110	2,700° (calcd.) ^[10] 2,700 °C ^[17]	
$p_{\text{C-J}}$ [kbar]	180		
VoD [m s ⁻¹]	6,763 (@ 1.62 g cm ⁻³)	6,800 (@ TMD, calcd., R-P method) ^[14] 6,850 (max. VoD) ^[17]	22,400 ft/s (@ 1.6 g cm ⁻³) ^[6] 6,850 (@ 1.62 g cm ⁻³) ^[7, 9, 12] 6,620 (@ 1.52 g cm ⁻³) ^[10] 6,850 (@ 1.68 g cm ⁻³) ^[10] 22,400 ft/s (@ 1.6 g/ml) ^[23]
V_0 [L kg ⁻¹]	657	675 ^[17]	844 ^[9] 675 ^[25]

Trauzl test [cm ³ , % TNT]	86–99% TNT ^[12] , 85% TNT ^[10] , 90% PA ^[10] , 275 cc ^[15] , 275 cm ³ (i.e., 90% PA) ^[17] , 384 cc (15 g sample) ^[18] , 290 cc ^[25] , 285 ^[26]
Ballistic mortar test	94% TNT ^[12]
5 s explosion T [°C] Explosion T [°C] 5 s ignition T [°C]	405 ^[10, 23] , 252–255 (heating rate = 10 °C/min) ^[10] , 275 ^[17] 270–276 ^[13]

Solubility [g/mL]	Less soluble in H ₂ O than PA ^[17] , 0.15 g dissolves in 100 g H ₂ O @ 6 °C ^[17] , 0.2 g dissolves in 100 g H ₂ O @ 15 °C ^[17] , 1.83 g dissolves in 100 g H ₂ O @ 100 °C ^[17] , 9.2 g dissolves in 100 g benzene @ 6 °C ^[17] , 13 g dissolves in 100 g benzene @ 15 °C ^[17] , readily soluble in EtOH, acetone, Et ₂ O ^[17, 18] , yellow needles recryst. from H ₂ O ^[18] , soluble in 449 parts H ₂ O @ 20 °C ^[18] , soluble in 123 parts H ₂ O @ 100 °C ^[18] , 0.15 parts dissolve per 100 parts H ₂ O (by wt.) @ 6 °C ^[25] , 0.20 parts dissolve per 100 parts H ₂ O (by wt.) @ 25 °C ^[25] , 1.83 parts dissolve per 100 parts H ₂ O (by wt.) @ 100 °C ^[25] , dissolves readily in EtOH, Et ₂ O, benzene and acetone ^[25]
Flash point [°C]	27(?)5 (unclear in original lit.) ^[25]
Brisance	4.2 mm (according to <i>Kast</i>) ^[25]
Manometric bomb	Gas pressure (exptl.) by exploding samples in small bombs, pressure measured by piston and obturator ^[16] : loading $\rho = 0.20 \text{ g cm}^{-3}$, pressure = 1,760 kg/cm ² ^[16] , loading $\rho = 0.25 \text{ g cm}^{-3}$, pressure = 2,480 kg/cm ² ^[16] , loading $\rho = 0.30 \text{ g cm}^{-3}$, pressure = 3,360 kg/cm ² ^[16]

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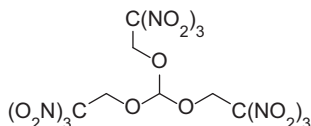
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2,2,2-Trinitroethyl formate

Name [German, acronym]: Trinitroethylformal, 2,2,2-trinitroethyl formate, trinitroethyl orthoformate, tri-2,2,2-trinitroethanol methane, tris(2,2,2-trinitroethyl)orthoformate [TNEF*, TTNEF, TNEOF]

Main (potential) use: Oxidizer, possible future chlorine-free oxidizer^[6]

Structural formula:



*TNEF is also used in the literature as the abbreviation for Trinitroethyl formal, $C_5H_5N_6O_{14}$

	TNEF
Formula	$C_7H_7N_9O_{21}$
Molecular mass [g mol ⁻¹]	553.2
Appearance at RT	Colorless rod-like crystals ^[5] , crude product is creamy colored ^[6, 7] , colorless crystals from dichloromethane ^[6, 7] , hexagonal rod crystals from dichloromethane ^[6]
IS [J]	5 (BAM) ^[1, 6] , $H_{50\%} = 7$ cm ^[2] , 5 (BAM, 50% initiation probability) ^[5] , 5.4 (BAM, crystals, 50% initiation probability) ^[6] , 4.6 (BAM, raw TTNEF) ^[7] , 7.8 (BAM, recryst. TTNEF) ^[7]
FS [N]	96 (BAM) ^[1, 6] , $H_{50\%} = 8$ cm (2.5 kg mass) ^[3] , 95 (BAM, 50% initiation probability) ^[5] , 92 (raw TTNEF, BAM) ^[7] , 106 (recryst. TTNEF BAM) ^[7]
ESD [J]	0.2 ^[1]
N [%]	22.8
$\Omega(CO_2)$ [%]	+10.1
$T_{m.p.}$ [°C]	128 ^[3] , 127.1 (DSC @ 5 °C/min, ~ 3 mg sample) ^[4] , 126.7 (small endo, DSC @ 5 °C/min) ^[5] , 122.7 (endo, onset), 127.1 (endo peak max) (DSC @ 5 K/min) ^[7]
$T_{dec.}$ [°C]	192 (DSC @ 5 °C/min) ^[1] , 210.1 (DSC @ 5 °C/min, ~ 3 mg sample) ^[4] , 210.2 (exo, DSC @ 5 °C/min) ^[5] , 189.6 (exo, onset), 210.1 (exo, peak max), 223.0 (end of dec.) (DSC @ 5 K/min) ^[7]

Data from^[4, 5]:

β (°C/min)	TG curve			DTG peak	
	T_{ot} (°C)	T_i (°C)	Mass loss (%)	T_p (°C)	T_{oe} (°C)
2.0	168.66	180.37	99.62	197.87	205.46
4.0	174.27	187.41	99.14	203.46	218.57
8.0	181.11	194.16	98.53	209.78	231.28
16.0	189.96	203.75	97.98	216.21	246.94

T_e = onset $T_{dec.}$, T_i = initial $T_{dec.}$, T_p = peak T , T_{oe} = onset T of the end decomposition

Data from^[6]:

β (K/min)	TG curve		DTG peak	
	T_o (°C)	Mass loss (%)	T_p (°C)	T_e (°C)
1.0	169.0	98.79	186.6	196.1
3.0	184.5	97.67	200.3	211.8
5.0	188.8	99.54	206.2	217.8
7.0	192.1	97.06	209.6	221.0

T_o = onset $T_{dec.}$, T_i = initial $T_{dec.}$, T_p = peak T , T_e = onset T of the end decomposition, T_p = peak T of mass loss rate; mass loss from initial T to end T of DTG peak (first) first dec. peak, (second) second dec. peak

Data from^[7]:

β (K/min)	TG curve			DTG peak	
	T_{ot} (°C)	T_i (°C)	Mass loss (%)	T_p (°C)	T_{oe} (°C)
1.0	170.8	182.3	98.6	186.6	188.9
3.0	184.9	193.5	96.8	200.3	205.1
5.0	190.7	202.6	99.1	206.2	210.9
7.0	195.3	206.8	95.0	209.6	218.3

T_e = onset $T_{dec.}$, T_i = initial $T_{dec.}$, T_p = peak T , T_{oe} = onset T of the end decomposition

ρ [g cm ⁻³]	1.81 (@ 298 K) ^[1, 4] , 1.83 (crystal) ^[3]
Heat of formation	-1,021 kJ/kg ^[1] , -140 kcal/mol (calcd.) ^[3] , -938.2 kJ/kg (enthalpy of form., ΔH) ^[4]

	Calcd. (EXPLO5 6.03)	AP for comparison
I_{sp} [s] (neat) ^a	228	-
I_{sp} [s] (neat) ^b	288	-
I_{sp} [s] ^{a,c} (71% oxidizer)	243	256
I_{sp} [s] ^{b,c} (71% oxidizer)	307	330

^a 70 bar/1 bar, isobaric combustion, equilibrium to throat and frozen to exit

^b 70 bar, 1 mbar, isobaric combustion, equilibrium to throat and frozen to exit

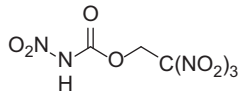
^c 15% Al; 6% polybutadiene acrylic acid, 6% polybutadiene acrylonitrile and 2% bisphenol A ether)

Burn rate [mm/s]	2.86 (TTNEF/HTPB cf. 2.70 for AP/HTPB) ^[6]																																												
Solubility [g/mL]	Can be recrystallized from dichloromethane ^[6] , soluble in acetone, CHCl ₃ and CH ₃ CN ^[7]																																												
Activation energy to decomposition [kJ/mol]	<p>198.4 (nonisothermal TGA, Kissinger method)^[4], 192.6 (mean value, nonisothermal, Ozawa Flynn-Wall, OFW method)^[5], 193–198 ± 0.4 (range of values, nonisothermal OFW method)^[5], 146.4 (TG-DTG, Kissinger method)^[6, 7], varied from step to step of conversion, mean value = 132.1 kJ/mol (OFW method)^[6], 131.5 ± 3.8 (KAS method)^[7]</p> <p>Modified KAS method, data from^[6, 7]:</p> <table><tr><td>α reacted</td><td>E_a</td><td>log A</td><td>r</td></tr><tr><td>0.1</td><td>123.8</td><td>12.08</td><td>0.9993</td></tr><tr><td>0.2</td><td>124.7</td><td>11.98</td><td>0.9989</td></tr><tr><td>0.3</td><td>127.3</td><td>12.15</td><td>0.9991</td></tr><tr><td>0.4</td><td>129.6</td><td>12.31</td><td>0.9986</td></tr><tr><td>0.5</td><td>131.6</td><td>12.45</td><td>0.9994</td></tr><tr><td>0.6</td><td>133.6</td><td>12.60</td><td>0.9988</td></tr><tr><td>0.7</td><td>135.4</td><td>12.72</td><td>0.9989</td></tr><tr><td>0.8</td><td>136.0</td><td>12.71</td><td>0.9991</td></tr><tr><td>0.9</td><td>135.5</td><td>12.55</td><td>0.9984</td></tr><tr><td>Mean</td><td>131.5</td><td>12.45</td><td></td></tr></table>	α reacted	E_a	log A	r	0.1	123.8	12.08	0.9993	0.2	124.7	11.98	0.9989	0.3	127.3	12.15	0.9991	0.4	129.6	12.31	0.9986	0.5	131.6	12.45	0.9994	0.6	133.6	12.60	0.9988	0.7	135.4	12.72	0.9989	0.8	136.0	12.71	0.9991	0.9	135.5	12.55	0.9984	Mean	131.5	12.45	
α reacted	E_a	log A	r																																										
0.1	123.8	12.08	0.9993																																										
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2,2,2-Trinitroethyl nitrocarbamate

Name [German, acronym]: 2,2,2-Trinitroethyl nitrocarbamate [TNC-NO₂, NTNC]
Main (potential) use: Halogen-free oxidizer
Structural formula:



	TNC-NO ₂	
Formula	C ₃ H ₃ N ₅ O ₁₀	
Molecular mass [g mol ⁻¹]	269.1	
Appearance at RT		
IS [J]	10 ^[1, 4]	
FS [N]	96 ^[1, 4]	
ESD [J]	0.1 ^[1]	
N [%]	26.0	
Ω(CO ₂) [%]	+14.9	
T _{m.p.} [°C]	109 ^[1] , 111.1 (endo, DSC @ 5 K/min) ^[4] , 111.4 (endo, DSC @ 10 K/min) ^[4] , 111.9 (endo, DSC @ 15 K/min) ^[4] , 111.7 (endo, DSC @ 20 K/min) ^[4]	
T _{dec.} [°C]	153 (DSC @ 5 °C/min) ^[1] , 157.8 (endo, DSC @ 5 K/min) ^[4] , 165.8 (endo, DSC @ 10 K/min) ^[4] , 173.2 (endo, DSC @ 15 K/min) ^[4] , 176.1 (endo, DSC @ 20 K/min) ^[4]	
ρ [g cm ⁻³]	1.73 (@ 298 K) ^[1]	
Heat of formation	−366 kJ/mol (Δ _f H°) ^[1] , −1,277 kJ/kg (Δ _f H°) ^[1]	
	Calcd. (EXPLO5 6.03)	AP for comparison
I _{sp} [s] (neat) ^a	226	--
I _{sp} [s] (neat) ^b	284	--
I _{sp} [s] ^{a,c} (71% oxidizer)	255	256
I _{sp} [s] ^{b,c} (71% oxidizer)	327	330

^a 70 bar/1 bar, isobaric combustion, equilibrium to throat and frozen to exit
^b 70 bar, 1 mbar, isobaric combustion, equilibrium to throat and frozen to exit
^c 15% Al; 6% polybutadiene acrylic acid, 6% polybutadiene acrylonitrile, and 2% bisphenol A ether)

Critical temperature of thermal explosion (T_b) [K]	479.54 ^[4]
Solubility [g/mL]	Soluble in CCl_4 ^[4]
Compatibility	<p>ΔT_p (dec. peak): NTNC/RDX = 2.1 °C < pure NTNC (good compatibility)^[4], ΔT_p (dec. peak): NTNC/DNAN = 25.0 °C < pure NTNC (bad compatibility)^[4], ΔT_p (dec. peak): NTNC/HTPB = 81.9 °C < pure NTNC (bad compatibility)^[4], NTNC reacts with centralite on grinding^[4]</p> <p>Compatibility: NTNC/boron (good) > NTNC/AP (good) > NTNC/NC (good) > NTNC/TNT (good) > NTNC/Al (good) > NTNC/RDX (good) > NTNC/NC + NG (moderate) > NTNC/CL-20 (poor) > NTNC/HMX (poor) > NTNC/Fox-7 (poor) > NTNC/DNAN (bad) > NTNC/HTPB (bad) > NTNC/centralite (bad)^[4]</p>

	TNC-NO₂ ^[1]
Chemical formula	$\text{C}_3\text{H}_3\text{N}_5\text{O}_{10}$
Molecular weight [g mol ⁻¹]	269.08
Crystal system	Monoclinic
Space group	$P2_1/c$ (no. 14)
a [Å]	10.784(2)
b [Å]	11.527(2)
c [Å]	8.752(2)
α [°]	90
β [°]	108.20(2)
γ [°]	90
V [Å ³]	1,033.5(7)
Z	4
ρ_{calc} [g cm ⁻³]	1.730(2)
T [K]	243

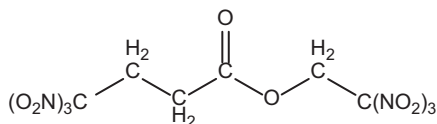
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Trinitroethyltrinitrobutyrate

Name [German, acronym]: 2,2,2-Trinitroethyl-4,4,4-trinitrobutyrate, butanoic acid 4,4,4-trinitro-, 2,2,2-trinitroethyl ester, 2,2,2-trinitroethyl 4,4,4-trinitrobutanoate [TNETB]

Main (potential) use: Melt-castable high explosive^[1], too sensitive to mechanical shock to be used as military explosive on its own^[2], high oxygen content explosive^[3], ingredient of composite explosives^[9]

Structural formula:



	TNETB
Formula	$C_6H_6N_6O_{14}$
Molecular mass [g mol ⁻¹]	386.14
Appearance at RT	Colorless solid ^[2] , white crystalline solid ^[3] , colorless crystalline solid ^[7]
IS [J]	$H_{50\%} = 20$ cm ^[3] , 18 cm (50% point, type 12 tool, 2.5 kg mass, sandpaper) ^[4] , 30 (<100 μm grain size, BAM) ^[7] , $H_{50} = 18$ cm ^[10]
FS [N]	240 (<100 μm grain size, BAM) ^[7]
ESD [J]	0.1 (100 μm grain size, BAM) ^[7]
N [%]	21.76
Ω(CO ₂) [%]	-4.2
$T_{m.p.}$ [°C]	93 ^[1, 3] , 92.5–93 (form II) ^[3] , 92 (DSC @ 5 °C/min) ^[7] , 93.50 (endo, DSC @ 5 °C/min) ^[9]
$T_{phase\ transition}$ [°C]	89 (form I → form II, solid → solid transition, irreversible @ 89 °C) ^[3] , RT (form II → form I, several hours) ^[3] , form III is stable over a very narrow temperature range (−0.2 → 0.3 °C) @ approx. 92.5 °C ^[3]

$T_{\text{dec.}} [^{\circ}\text{C}]$	155 (DSC @ 5 $^{\circ}\text{C}/\text{min}$) ^[7] , 204 (exo, peak max., DSC @ 5 $^{\circ}\text{C}/\text{min}$) ^[9] Data from ^[9] : <table data-bbox="379 287 1044 513"> <tr> <th>β (K/min)</th><th>T_0 (K)</th><th>T_e (K)</th><th>T_p (K)</th></tr> <tr> <td>2.09</td><td>401.15</td><td>419.15</td><td>468.15</td></tr> <tr> <td>5.24</td><td>411.15</td><td>429.15</td><td>477.15</td></tr> <tr> <td>10.77</td><td>423.15</td><td>441.15</td><td>491.15</td></tr> <tr> <td>22.14</td><td>437.15</td><td>454.15</td><td>504.95</td></tr> </table>			β (K/min)	T_0 (K)	T_e (K)	T_p (K)	2.09	401.15	419.15	468.15	5.24	411.15	429.15	477.15	10.77	423.15	441.15	491.15	22.14	437.15	454.15	504.95
β (K/min)	T_0 (K)	T_e (K)	T_p (K)																				
2.09	401.15	419.15	468.15																				
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10.77	423.15	441.15	491.15																				
22.14	437.15	454.15	504.95																				
ρ [g cm ⁻³]	1.78 (form I) ^[3] , 1.783 (loading density, form I) ^[3] , 1.677 (loading density, form II) ^[3] , 1.551 (liquid @ 99 $^{\circ}\text{C}$) ^[3] , 1.84 (crystal) ^[9]																						
Heat of formation	307 cal/g ^[3] , -496.2 kJ/mol (enthalpy of form.) ^[6] , -421.7 kJ/mol (enthalpy of form., calcd., emp.) ^[6] , -530.3 kJ/mol (enthalpy of form., calcd. S-D method) ^[6] , 118.6 kcal/mol ^[8] , -495.80 kJ/mol (standard enthalpy of form. (Q_f)) ^[9]																						
Heat of combustion	1,685 cal/g ^[3] , 1.620 kcal/g ^[8] , -2,722.75 \pm 0.79 kJ/mol (standard combustion enthalpy, $\Delta_c H_m^{\circ}$) ^[9] , -2,743.82 \pm 0.79 kJ/mol (standard combustion energy, $\Delta_c U$) ^[9]																						
	Calcd. (EXPLO5 6.02)	Lit. values	Exptl.																				
$-\Delta_{\text{ex}} U^{\circ}$ [kJ kg ⁻¹]	-6,121	Heat of detonation = 1.45 kcal/g ^[8]																					
T_{ex} [K]	4,277																						
$p_{\text{C-J}}$ [kbar]	335																						
VoD [m s ⁻¹]	8,616	5,960 (@ 1 g cm ⁻³ , calcd., Kamlet method) ^[1] 7,990 (@ 1.6 g cm ⁻³ , calcd., Kamlet method) ^[1] 5,410 (@ 1 g cm ⁻³ , calcd., Urizar method) ^[1] 7,760 (@ 1.6 g cm ⁻³ , calcd., Urizar method) ^[1] 8,362 (@ 1.774 g cm ⁻³) ^[9]	5,610 (@ 1 g cm ⁻³) ^[1] 7,800 (@ 1.6 g cm ⁻³) ^[1] 7,760 (@ 1.60 g cm ⁻³) ^[3] 8,290 (@ 1.76 g cm ⁻³) ^[3]																				
V_0 [L kg ⁻¹]	719																						

t_{sp} [s]	258 (pure TNETB, 70.0 bar chamber pressure, isobaric combustion conditions (1 bar), equilibrium expansion) 263 (TNETB with 15% Al, 70.0 bar chamber pressure, isobaric combustion conditions (1 bar), equilibrium expansion) 255 (71% TNETB, 15% Al, 14% binder (6% polybutadiene acrylic acid, 6% polybutadiene acrylonitrile, 2% bisphenol A ether 70.0 bar chamber pressure, isobaric combustion conditions (1 bar), equilibrium expansion)																																								
Critical T of thermal explosion, T_b [K]	426.05 ^[9] , 478.47 ^[9] , 422.49 ^[9] , 476.79 ^[9] , 426.02 ^[9] , 477.88 ^[9] , 426.17 ^[9] , 478.13 ^[9] , 408.90 ^[9] , 406.24 ^[9]																																								
Ballistic mortar test	136% TNT ^[3]																																								
LSGT [cm]	$\rho = 1.64 \text{ g/cm}^3$ (cast), 92.6% TMD, 50% point = 277 cards ^[5]																																								
SSGT [cm]	(1) = no mixed response zone, data from ^[4] : <table><tr><td>Loading pressure (kpsi)</td><td colspan="2">Density (g/cm³)</td><td>% TMD</td><td colspan="4">Sensitivity (DBG)</td></tr><tr><td></td><td>AVG.</td><td>s</td><td></td><td>AVG.</td><td>g</td><td>s_m</td><td>N</td></tr><tr><td>8</td><td>1.563</td><td>0.0088</td><td>87.3</td><td>3.042</td><td>-</td><td>-</td><td>23(1)</td></tr><tr><td>16</td><td>1.698</td><td>0.0046</td><td>94.9</td><td>4.193</td><td>0.0530</td><td>0.0306</td><td>23</td></tr><tr><td>32</td><td>1.776</td><td>0.0023</td><td>99.2</td><td>5.497</td><td>0.0016</td><td>0.0022</td><td>23</td></tr></table>	Loading pressure (kpsi)	Density (g/cm ³)		% TMD	Sensitivity (DBG)					AVG.	s		AVG.	g	s_m	N	8	1.563	0.0088	87.3	3.042	-	-	23(1)	16	1.698	0.0046	94.9	4.193	0.0530	0.0306	23	32	1.776	0.0023	99.2	5.497	0.0016	0.0022	23
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	AVG.	s		AVG.	g	s_m	N																																		
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32	1.776	0.0023	99.2	5.497	0.0016	0.0022	23																																		
5 s explosion T [°C]	225 (50% point, Alhot bar) ^[3]																																								
Vacuum stability test [cm ³ /h]	0.60 cc/48 h @ 100 °C ^[3]																																								
Vapor pressure [atm. @ °C]	Values from ^[3] : <table><tr><td>T (°C)</td><td>mm Hg</td></tr><tr><td>65</td><td>3.3×10^{-5}</td></tr><tr><td>75</td><td>1.3×10^{-4}</td></tr><tr><td>100</td><td>2.3×10^{-3}</td></tr><tr><td>120</td><td>1.4×10^{-2}</td></tr></table>	T (°C)	mm Hg	65	3.3×10^{-5}	75	1.3×10^{-4}	100	2.3×10^{-3}	120	1.4×10^{-2}																														
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100	2.3×10^{-3}																																								
120	1.4×10^{-2}																																								
Viscosity [Poises]	Absolute viscosity = 0.173 Poises @ 98.9 °C ^[3] , absolute viscosity = 0.138 Poises @ 106.5 °C ^[3]																																								

Solubility [g/mL]	<p>Insoluble in H₂O, <i>n</i>-hexane and CCl₄^[2], very soluble in nitromethane, glacial acetic acid and ethyl acetate^[2], recryst. from water/MeOH or CHCl₃^[7], recryst. from nitromethane^[9]</p> <p>Solubility at room temperature^[3]:</p> <table border="1" data-bbox="381 351 1041 793"> <thead> <tr> <th>Solvent</th><th>Solubility</th></tr> </thead> <tbody> <tr> <td>Water</td><td>Insoluble</td></tr> <tr> <td><i>n</i>-Hexane</td><td>Insoluble</td></tr> <tr> <td>CCl₄</td><td>Insoluble</td></tr> <tr> <td>EtOH</td><td>5 g/100 g solvent</td></tr> <tr> <td>CHCl₃</td><td>5 g/100 g solvent</td></tr> <tr> <td>Benzene</td><td>10 g/100 g solvent</td></tr> <tr> <td>Nitromethane</td><td>Very soluble</td></tr> <tr> <td>Glacial acetic acid</td><td>Very soluble</td></tr> <tr> <td>Ethyl acetate</td><td>Very soluble</td></tr> </tbody> </table> <p>TNETB forms eutectics with the following: TNT 57^[3], BTNES (bis(trinitroethyl) succinate) 80 +^[3], BTNEN (bis(trinitroethyl) nitramine) 68.5^[3], TNB (trinitrobenzene) 65^[3], trinitroethyl trinitrobenzoate (27%) 80.5^[3]</p>	Solvent	Solubility	Water	Insoluble	<i>n</i> -Hexane	Insoluble	CCl ₄	Insoluble	EtOH	5 g/100 g solvent	CHCl ₃	5 g/100 g solvent	Benzene	10 g/100 g solvent	Nitromethane	Very soluble	Glacial acetic acid	Very soluble	Ethyl acetate	Very soluble
Solvent	Solubility																				
Water	Insoluble																				
<i>n</i> -Hexane	Insoluble																				
CCl ₄	Insoluble																				
EtOH	5 g/100 g solvent																				
CHCl ₃	5 g/100 g solvent																				
Benzene	10 g/100 g solvent																				
Nitromethane	Very soluble																				
Glacial acetic acid	Very soluble																				
Ethyl acetate	Very soluble																				
Hygroscopicity	0% @ 75 °C, 90% RH, 5 months ^[3]																				
Refractive index	Form I, crystal axis α $n_{20}^D = 1.518$ ^[3] , crystal axis β $n_{20}^D = 1.527$ ^[3] , crystal axis γ $n_{20}^D = 1.546$ ^[3]																				
ΔH_{sub} [cal/g]	Heat of sublimation = 804 (est.) ^[3]																				
Bruceton safety test results	Mean and standard deviation of lengths of 0.300 diameter cylinder across which initiation is possible for 50% certainty: TNT = 0.391 ± 0.040 ^[3] , RDX Comp B = 0.381 ± 0.042 ^[3] , TNETB = 0.920 ± 0.059 ^[3]																				
Specific heat capacity, C_p	1.10 J (g K ⁻¹) (calcd.) ^[9]																				
Thermal conductivity, λ	0.2218 W (m K) ⁻¹ ^[9]																				
Self-accelerating decomposition T , T_{SADT} [K]	410.92 ^[9]																				

	TNETB^[7]
Chemical formula	C ₆ H ₆ N ₆ O ₁₄
Molecular weight [g mol ⁻¹]	386.14
Crystal system	Monoclinic
Space group	<i>P</i> 2 ₁ / <i>n</i> (14)
<i>a</i> [Å]	5.7264(3)
<i>b</i> [Å]	21.6530(11)
<i>c</i> [Å]	11.0910(6)
α [°]	90
β [°]	93.555(4)
γ [°]	90
<i>V</i> [Å ³]	1,372.57(12)
<i>Z</i>	4
ρ_{calc} [g cm ⁻³]	1.869
<i>T</i> [K]	100
	Recryst. from CHCl ₃

*3 polymorphic crystalline forms have been observed

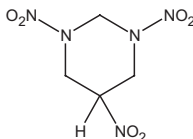
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1,3,5-Trinitrohexahydropyrimidine

Name [German, acronym]: 1,3,5-Trinitrohexahydropyrimidine [TNP]

Main (potential) use: academic

Structural formula:



	TNP		
Formula	$\text{C}_4\text{H}_7\text{N}_5\text{O}_6$		
Molecular mass [g mol ⁻¹]	221.1		
Appearance at RT	Sparkling white plate crystals ^[2]		
IS [J]	$H_{50\%} > 100 \text{ cm}^{[2]}$		
FS [N]	Insensitive up to 36 kg load ^[2]		
N [%]	31.67		
$\Omega(\text{CO}_2)$ [%]	-39.8		
$T_{\text{m.p.}}$ [°C]	DSC (@ 10 °C/min: endo dip directly before exotherm @ 147 °C) ^[1] , 140–142 ^[2]		
$T_{\text{dec.}}$ [°C]	DTA (@ 10 °C/min, static air atmosphere): 144–163 (exo, peak max. @ 149 °C), broad exo max. @ 272 °C ^[1] , DTA (@ 10 °C/min, N ₂ atmosphere): 146–178 (exo, exo peak max @ 168 °C) ^[1] , DSC (@ 10 °C/min): exo one stage dec. @ 147–163 (peak max @ 155, onset = 149) ^[1] , isoDTA: dominant sharp exo @ 120 ^[1] , 142–160 (75% wt. loss) and 160–500 (14% wt. loss) (2 stage dec., TG) ^[2]		
ρ [g cm ⁻³]	1.78 ^[2]		
Heat of formation	40.08 kJ/mol (ΔH_f) ^[2]		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^\circ$ [kJ kg ⁻¹]			
T_{ex} [K]			
p_{C_1} [kbar]		30.02 (@ 1.78 g cm ⁻³ , calcd., LOTUSES) ^[2]	

VoD [m s^{-1}]		8,091 (@ 1.78 g cm^{-3} , calcd., LOTUSES) ^[2]	
V_0 [L kg^{-1}]		1,068 (@ 1.78 g cm^{-3} , calcd., LOTUSES) ^[2]	
Thermal stability	<p>TG (static air): 76% weight loss in range 142–150 °C, 12% slow weight loss in range 150–448 °C^[1]</p> <p>TG (dynamic nitrogen): change in weight = 71% in range 146–171 °C^[1]</p> <p>IsoTG (under static air): no weight loss in 400 min <108 °C, 6.1% weight loss in 290 min @ 109 °C, 18% weight loss in 260 min @ 115 °C, 35.5% weight loss in 320 min @ 118 °C; @ 120 °C after ~ 12% weight loss in 80 min a sudden weight loss of 78% occurred^[1]</p>		

	TNP^[1]
Chemical formula	$\text{C}_4\text{H}_7\text{N}_5\text{O}_6$
Molecular weight [g mol^{-1}]	221.1
Crystal system	Hexagonal
Space group	
a [Å]	18.818 ± 0.005
b [Å]	18.818 ± 0.005
c [Å]	4.867 ± 0.005
α [°]	
β [°]	
γ [°]	
V [Å ³]	
Z	
ρ_{calc} [g cm^{-3}]	
T [K]	
	Powder diffraction

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Trinitromethane

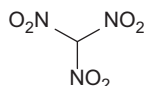
Name [German, acronym]:

Trinitromethane, nitroform

Main (potential) use:

Starting material for HEDOs

Structural formula:



	Nitroform
Formula	CHN ₃ O ₆
Molecular mass [g mol ⁻¹]	151.03
Appearance at RT	Brown, volatile liquid ^[8] , colorless crystalline ^[9] , colorless crystalline substance with characteristically sharp odor ^[10] , colorless nitroform turns yellow on absorption of moisture ^[10] , dry crystals are white ^[11]
IS [J]	$H_{50\%} = 218$ cm (1 kg mass, BRL apparatus) ^[5]
<i>N</i> [%]	27.82
Ω(CO ₂) [%]	+37.08
<i>T</i> _{m.p.} [°C]	25.4 ^[1] , 22 ^[4, 8] , 26.3 ^[5] , 26.4 ^[9] , 23–25 ^[10] , 15 ^[11] , 50 (unstable <i>aci</i> -form) ^[11]
<i>T</i> _{b.p.} [°C]	48 ^[8] , 45–47 (@ 22 mm Hg) ^[10]
<i>T</i> _{dec.} [°C]	dec. >25 ^[11]
<i>ρ</i> [g cm ⁻³]	1.806 ^[2] , 1.479 ^[4] , 1.5967 (@ 24.3 °C) ^[5] , 1.59 ^[8] , sp. gr. $d_{40}^{25} = 1.61$ ^[10] , $d_4^{25}(\text{liq.}) = 1.469$ ^[11]
Heat of formation	–68.0 ± 3.1 kJ/mol ($\Delta_f H^\circ(\text{liq.})$) ^[3] , –32.1 kJ/mol ($\Delta_f H^\circ(\text{liq.})$) ^[3] , –77.95 kJ/mol ($\Delta_f H^\circ(\text{liq.})$) ^[3] , –48.0 ± 2.0 kJ/mol ($\Delta_f H^\circ(\text{s})$) ^[3] , –38.58 kJ/mol (standard heat of form.) ^[4] , –255.46 kJ/kg (standard heat of form.) ^[4] , 4.2 kcal/mol ($\Delta_f H^\circ(\text{g})$ °, calcd., ccCA-P) ^[12] , 1.2 kcal/mol ($\Delta_f H^\circ(\text{g})$ °, calcd., ccCA-S3) ^[12] , 2.7 kcal/mol ($\Delta_f H^\circ(\text{g})$ °, calcd., ccCA-PS3) ^[12] , 0.6 kcal/mol ($\Delta_f H^\circ(\text{g})$ °, calcd., G3) ^[12] , 5.4 kcal/mol ($\Delta_f H^\circ(\text{g})$ °, calcd., G3(MP2)) ^[12] , –5.7 ± 0.3 kcal/mol ($\Delta_f H^\circ(\text{g})$ °, exptl.) ^[12]
Heat of combustion [cal/g]	$\Delta_c H^\circ(\text{l}) = -504.30$ kJ/mol ^[3] , $\Delta_c H^\circ(\text{l}) = -458.48$ kJ/mol ^[3] , $\Delta_c H^\circ(\text{s}) = -488.0 \pm 13.0$ kJ/mol ^[3] , heat of comb. = 746 cal/g ^[11]

	Calcd. (EXPLO5 6.03)	Exptl.
$-\Delta_{\text{ex}}U^{\circ}$ [kJ kg ⁻¹]	3,009	3,120 ^[4]
T_{ex} [K]	2,839	
$p_{\text{C-J}}$ [kbar]	215	
VoD [m s ⁻¹]	7,486	
V_0 [L kg ⁻¹]	764	

Trauzl test [cm ³ , % TNT]	~100% TNT ^[6]
Ballistic mortar test	125–137% TNT ^[5]
Initiation efficiency	Can be detonated by shock or a capsule ^[10]
5 s explosion T [°C]	Explodes on rapid heating ^[10]
Thermal stability	Explodes on rapid heating ^[10, 11] , can be distilled without dec. ^[10]
Solubility [g/mL]	Forms azeotropic mixture with nitric acid ^[8] , readily soluble in water and common organic solvents ^[10] , solns. of nitroform in H ₂ O, EtOH, acetic acid and aqueous Et ₂ O are yellow ^[10] , solns. in benzene, CHCl ₃ , CS ₂ , ligroin, Et ₂ O and in conc. hydrochloric or sulfuric acids are colorless ^[10] , soluble in water forming an intensely yellow soln. ^[11]
Hygroscopicity	Readily absorbs moisture and turns yellow ^[10]
ΔH_{sub} [kJ/mol]	45.2 (exptl.) ^[7] , 71.5 (calcd., QSPR) ^[7]
Acidity	Very strong acid ^[10]
Dipole moment	2.61 (benzene) ^[11]

	Nitroform ^[2]
Chemical formula	CHN ₃ O ₆
Molecular weight [g mol ⁻¹]	151.05
Crystal system	Cubic
Space group	<i>Pa</i> -3 (no. 205)
a [Å]	10.3580(10)
b [Å]	10.3580(10)
c [Å]	10.3580(10)
α [°]	90

β [°]	90
γ [°]	90
V [Å ³]	1,111.3
Z	8
ρ_{calc} [g cm ⁻³]	1.806
T [K]	200

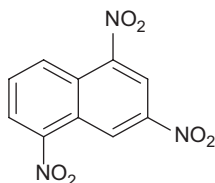
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Trinitronaphthalene

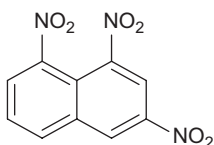
Name [German, acronym]: Trinitronaphthalene, naphtite [trinitronaphthalin, trinal, TN, TNN]

Main (potential) use: Was used in mixtures with other explosives in the past^[8], filling shells, usually in fusible mixtures with TNT^[16]

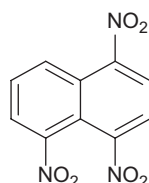
Structural formula:*



1,3,5-TNN
alpha-TNN



1,3,8-TNN
beta-TNN



1,4,5-TNN
gamma-TNN

* The crude and commercial products usually contain a mixture of the three isomers shown above^[16]; Commercial trinitronaphthalene is a mixture of the 1,3,5-, 1,4,5- and 1,3,8- isomers – the ratio of the isomers depends on the temperature and nitrating agent used^[18]

	TNN
Formula	$C_{10}H_5N_3O_6$
Molecular mass [g mol ⁻¹]	263.17
Appearance at RT	Very fine crystalline solid, light brownish-gray ^[16] , brownish solid (commercial) ^[18] , glittering yellow platelet crystals (1,4,5-) ^[20]
IS [J]	19 Nm ^[8] , 9.52 (drop energy, Julius-Peters, 1,4,5-isomer) ^[9] , similar to TNT (1,3,8-isomer) ^[10]
ESD [J]	10.97 ^[5] , 210.0 mJ ^[5] , 10.97 (1,4,5-TNN) ^[6, 22] , 9.25 cal (1,4,5-, calcd.) ^[18]
N [%]	15.97
Ω(CO ₂) [%]	−100.32
T _{m,p.} [°C]	120 (1,3,5-TNN) ^[1] , 217 (1,3,8-TNN) ^[1] , 148 (1,4,5-TNN) ^[1] , 122–123 (1,3,5-TNN) ^[10] , 223 (1,3,8-TNN) ^[10] , 147–149 (1,4,5-TNN) ^[10] , 123 (1,3,5-TNN) ^[16] , 218 (1,3,8-TNN) ^[16] , 147 (1,4,5-TNN) ^[16] , 115–160 (crude product, mixture of isomers) ^[16] , 115 (softening of the isomer mixture begins) ^[8] , 115 (commercial) ^[18] , 218 (1,3,5-) ^[20] , 147 (1,4,5-) ^[20] , 218 (1,3,8-) ^[20] , 112–113 (1,2,5-) ^[20]
T _{dec.} [°C]	1,3,5-TNN explodes @ 364 °C when heated in glass tube ^[10]

ρ [g cm ⁻³]	1.654 (@ 293 K, 1,3,5-TNN) ^[2] , 1.72–1.75 (@ 293 K, 1,3,8-TNN) ^[3] , 1.42 (crystal) ^[10] , 1.654 (@ 293 K, 1,4,5-TNN) ^[2]		
Heat of formation	–8.49 kJ/mol ($\Delta_f H^\circ$ (s), 1,3,8-TNN) ^[4] , –27 cal/g (Q_f^P , 1,3,8-TNN) ^[10] , –11 cal/g (Q_f^V , 1,3,8-TNN) ^[10] , –44.7 kcal/kg (1,3,8-) ^[19] , –55.5 kcal/kg (1,4,5-) ^[19] , –8.49 kJ/mol (enthalpy of form., exptl., 1,3,8-) ^[21] , 9.7 kJ/mol (enthalpy of form., calcd., emp., 1,3,8-) ^[21] , 30.0 kJ/mol (enthalpy of form., calcd., S-D method, 1,3,8-) ^[21]		
Heat of combustion	$\Delta_c H^\circ$ (s) = –4,673.9 ± 4.6 kJ/mol (1,3,8-TNN) ^[4] , $\Delta_c H^\circ$ (s) = –4,641.23 kJ/mol (1,3,8-TNN) ^[4] , $\Delta_c H^\circ$ (s) = –4,686.1 ± 4.6 kJ/mol (1,4,5-TNN) ^[4] , –1,190 kcal mol ⁻¹ (Q_c^P ; 1,3,8-TNN) ^[10] , –4,223.9 cal/g (Q_c^V ; 1,3,8-TNN) ^[10] , –1,122.7 kcal/mol (Q_c^P ; 1,4,5-TNN) ^[10] , 4,259 kcal/kg (1,3,8-, @ C°) ^[19] , 4,270 kcal/kg (1,4,5-, @ C°) ^[19]		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
	1,3,8-TNN		
$-\Delta_{\text{ex}} U^\circ$ [kJ kg ⁻¹]	3,734		3,521 [H ₂ O (l)] ^[7, 8] 3,425 [H ₂ O (g)] ^[8] 923 kcal/kg (isomer not specified) ^[20] 3,521 kJ/mol (1,3,5-, heat of detonation) ^[18]
T_{ex} [K]	2,780		
p_{C_1} [kbar]	160		19.32 GPa (1,4,5-) ^[18]
VoD [m s ⁻¹]	6,371 (@ 1.75 g cm ⁻³ , $\Delta_f H = -8.49$ kJ mol ⁻¹)	5,690 (@ TMD, calcd., R - P method) ^[15] 5,140 (max. VoD) ^[16]	6,000 (no density given) ^[8]
V_0 [L kg ⁻¹]	548		723 ^[8]

Trauzl test [cm ³ , % TNT]	166 cc (15 g sample) ^[17]
Ballistic mortar test	83% TNT (1,3,8-TNN) ^[11]
5 s explosion T [°C] Deflagration T [°C]	350 (commercial) ^[18]

Thermal stability	1,3,5-TNN @ 135 °C: no fumes after 30 min ^[10] , no explosion <360 °C ^[10]
Vacuum stability test [cm ³ /h]	1,3,8-TNN: 0.46 cc gas evolved per 5 mL sample in 48 h @ 120 °C ^[10]
Solubility [g/mL]	Sparingly soluble in common organic solvents ^[16] , 1,3,5- poorly soluble in EtOH ^[16] , 1,3,8- soluble in hot 70% EtOH ^[16] , 1,4,5- insoluble in 70% EtOH ^[16] , soluble in acetic acid, CHCl ₃ and EtOH (1,3,5-) ^[20] , soluble in EtOH (1,3,8-) ^[20] , weakly soluble in Et ₂ O and CHCl ₃ (1,3,8-) ^[20] , readily soluble in benzene (1,4,5-) ^[20] , weakly soluble in Et ₂ O, EtOH and CHCl ₃ (1,4,5-) ^[20] , readily soluble in EtOH (1,2,5-) ^[20]
Manometric bomb	Gas pressure (exptl.) by exploding samples in small bombs, pressure measured by piston and obturator ^[12] : loading $\rho = 0.25 \text{ g cm}^{-3}$, pressure = 2,045 kg/cm ² ^[12] , loading $\rho = 0.30 \text{ g cm}^{-3}$, pressure = 2,670 kg/cm ² ^[12]

Explosive properties of mixtures of trinitronaphthalene from ^[20]:

formula	*Sensitivity (weight = 10 kg, height = 25 cm) in % explosions	Trauzl fugacity (TNT, No. 8 cap) in cc	Brisance (no. 8 cap) in mm		Detonation velocity (m/s)	Pilling density (g/cm ³)
			Kast	Hess		
Technical TNN (mpt. = 150°)	12	228	2.16	—		1.43
16.3% TNN & 83.7% AN	18	106	3.95	7.6	5,610	1.6, 0.74
33% TNN & 66.4% AN	21	374	—	7.5	—	0.74 Hess test
35% TNN & 65% TNT (freezing point = *)	4	285	3.11		—	1.58
15% TNN & 85% TNT (freezing point = 74°)	1*	*	3.28		—	*
40% TNN & 60% trinitrophenol (freezing point = 82°)	1*	200	3.39	—	—	1.62
20% TNN & 80% trinitrophenol (freezing point = 105°)	12	312	3.72	—	—	1.63

* = illegible in original report

	1,3,5-TNN^[14, 20]	1,3,8-TNN^[3]	1,3,8-TNN^[13]
Chemical formula	C ₁₀ H ₅ N ₃ O ₆	C ₁₀ H ₅ N ₃ O ₆	C ₁₀ H ₅ N ₃ O ₆
Molecular weight [g mol ⁻¹]	263.17	263.17	263.17
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group		<i>P</i> 2 ₁ / <i>n</i> (no. 14)	<i>P</i> 2 ₁ / <i>n</i> (no. 14)
<i>a</i> [Å]		16.19	8.4353(13)
<i>b</i> [Å]		7.60	7.7114(14)
<i>c</i> [Å]		8.42	16.250(6)
α [°]		90	90
β [°]		99.27	99.57(3)
γ [°]		90	90
<i>V</i> [Å ³]		1,022.5	1,042.3(5)
<i>Z</i>		4	4
ρ_{calc} [g cm ⁻³]		1.71	1.677
<i>T</i> [K]		295	297

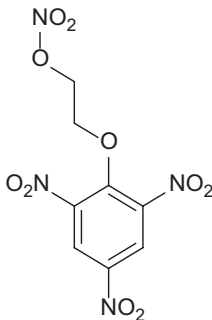
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Trinitrophenoxyethyl nitrate

Name [German, acronym]: 2-(2,4,6-Trinitrophenoxy)ethylnitrate,
trinitrophenoxyethyl- ω -nitrate,
 β -2,4,6-trinitrophenoxyethyl nitrate
[trinitrophenylglykolethernitrat, TNPON]
Main (potential) use: melt-cast

Structural formula:



	Trinitrophenoxyethyl nitrate
Formula	C ₈ H ₆ N ₄ O ₁₀
Molecular mass [g mol ⁻¹]	318.15
Appearance at RT	White crystalline powder ^[10] , white powder ^[11] , yellow-white crystals ^[7]
IS [J]	7.9 Nm ^[7]
N [%]	17.61
$\Omega(\text{CO}_2)$ [%]	-45.26
$T_{\text{m.p.}}$ [°C]	104 ^[1] , 104.5 ^[7, 10, 11]
$T_{\text{dec.}}$ [°C]	>300
ρ [g cm ⁻³]	1.723 ^[2] , 1.68 ^[7]
Heat of formation	-277.4 kJ/mol ($\Delta_f H^\circ$) ^[4] , -871.9 kJ/kg (enthalpy of form.) ^[7] , -277.3 kJ/mol (enthalpy of form., exptl.) ^[13] , -246.7 kJ/mol (enthalpy of form., calcd., emp.) ^[13] , -286.6 kJ/mol (enthalpy of form., calcd., S-D method) ^[13]

	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^\circ$ [kJ kg ⁻¹]	4,892		3,911 [H ₂ O (l)] ^[4] 3,473 [H ₂ O (g)] ^[6] 3,792 [H ₂ O (g)] ^[7]
T_{ex} [K]	3,530		
$p_{\text{C-J}}$ [kbar]	241		
VoD [m s ⁻¹]	7,561	7,290 (@ TMD, calcd., R-P method) ^[9]	7,600 (@ 1.68 g cm ⁻³) ^[3] 7,600 (@ 1.65 g cm ⁻³) ^[7]
V_0 [L kg ⁻¹]	662		878 ^[5, 7]

Trauzl test [cm ³ , % TNT]	122% TNT ^[8] , 350 cm ³ ^[12] , 350 cm ³ (10 g sample) ^[7]
Solubility [g/mL]	Soluble in acetone ^[7, 10] , insoluble in H ₂ O ^[7, 11] , readily soluble in acetone ^[11] , soluble in toluene ^[7]

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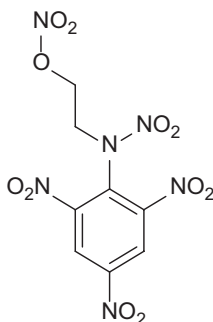
2,4,6-Trinitrophenylnitraminoethyl nitrate

Name [German, acronym]: 2,4,6-Trinitrophenylnitraminoethyl nitrate,
2-(2',4',6'-trinitro-*N*-nitroanilino)ethanol nitrate,
2,4,6-trinitro-1-(β -nitroxyethylnitroamino)-
benzene, trinitrophenylethanolnitramine nitrate
[trinitrophenylethanolnitraminnitrat, pentryl]

Main (potential) use:

Proposed as a base charge in detonators^[8]

Structural formula:



	Petryl
Formula	$C_8H_6N_6O_{11}$
Molecular mass [g mol ⁻¹]	362.17
Appearance at RT	Yellowish crystals ^[3] , yellowish, nearly white crystals ^[8]
IS [J]	4 Nm ^[3] , $H_{50\%} = 0.75$ m (2 kg mass) ^[4] , FI = 61% PA ^[4] , 0.26 m (5 kg mass, $H_{56\%}$) ^[4] , max. drop heights for no explosion = 30 cm (2 kg mass) ^[4, 7] , 0.02 g exploded by 2 kg dropped from 30 cm ^[5]
<i>N</i> [%]	23.21
$\Omega(\text{CO}_2)$ [%]	-35.34
$T_{m.p.}$ [°C]	129 ^[1] , 128 ^[3, 8] , 126–129 ^[4] , 126 ^[6]
$T_{dec.}$ [°C]	Explosion @ 235 °C (20 °C/min heating rate) ^[4] , explosion @ 230 °C (20 °C/min heating rate) ^[4]
ρ [g cm ⁻³]	1.858 ^[2] , 1.75 ^[3] , 1.82 (absol.) ^[4, 5] , 0.45 (apparent) ^[4, 5] , 1.73 (max by compression) ^[4] , 0.74 (apparent ρ when compressed in detonator shell @ 3,400 lb/in ²) ^[5] , sp. gr. = 1.82 ^[8]
Heat of formation	24.84 kcal/mol ($-\Delta H_f$, heat of form. @ standard conditions) ^[10]

Heat of combustion	Exptl. heat of combustion data ^[10] :			
	$-\Delta U_{B/M}$ (cal/g)	$-\Delta U_B$ (kcal/mol)	$-\Delta U_R$ (kcal/mol @ 1 atm. and constant vol.)	$-\Delta H_R$ (kcal/mol @ 1 atm. and constant pressure)
	2,600.70 \pm 1.22	941.05	940.05	935.91
	Calcd. (EXPLO5 5.04)	Lit. values	Exptl.	
$-\Delta_{\text{ex}}U^o$ [kJ kg ⁻¹]		372.4 kcal/mol (Q_e^V , calcd.) ^[3]		
T_{ex} [K]				
p_{C-J} [kbar]				
VoD [m s ⁻¹]			5,000 (@ 0.80 g cm ⁻³ in light Pb tube, >0.5 m length, 0.5 in) ^[4] 5,254 (@ 1.0 g cm ⁻³ , confined in ³ / ₁₆ in glass tube) ^[4] 5,330 (@ 0.90 g cm ⁻³ , cardboard cartridges, 30 mm diameter, initiated by 1.5 g MF) ^[4] 5,560 (@ 0.99 g cm ⁻³ , cardboard, 30 mm, 1.5 g MF) ^[3] 7,340 (@ 1.65 g cm ⁻³ , cardboard, 30 mm, 1.6 g MF) ^[3] 17,250 ft/s (@ 1.0 g/mL) ^[6] 5,000 (@ 0.8 g cm ⁻³) ^[8]	
V_o [L kg ⁻¹]				

Trauzl test [cm ³ , % TNT]	15.8 cc (small Trauzl test) ^[5, 7] , rel. strength cf. TNT = 1.30 ^[7, 8] , rel. strength cf. Tetryl = 1.15 ^[8] , rel. strength cf. PA = 1.27 ^[8] , 450 cm ³ ^[9] , 450 cm ³ (10 g sample) ^[3]
Lead block test	18.5 mm shortening of block (50 g Pentryl) ^[5]
Sand test [g]	129% TNT ^[3] , 67.5 g (amount of sand crushed finer than 30 mesh, by total charge consisting of base charge of 0.50 g Pentryl and 0.30 g priming charge of MF) ^[7] , 55.8 g (amount of sand crushed finer than 30 mesh, by base charge of 0.50 g Pentryl) ^[7] , rel. strength cf. TNT = 1.28 ^[7]
Initiation efficiency	Minimum weight of priming charge which causes complete detonation of the base charge ^[7] : 0.095 g DDNP ^[7] , 0.150 g MF ^[7] , 0.025 g LA ^[7]
5 s explosion <i>T</i> [°C] 3 s explosion <i>T</i> [°C] Explosion <i>T</i> [°C]	235 ^[5] 235 (ignition in 3 s, Wood's preheated bath) ^[3] , 250 (2 s) ^[3] , 270–280 (1.5 s) ^[3] , 235 ^[6, 8]
Thermal stability	Storage at moderately elevated <i>T</i> causes no loss in power ^[6] , storage under water causes no loss in power ^[6]
Burn rate [mm/s]	Burns without explosion when ignited without confinement ^[6]
Solubility [g/mL]	Some solubility in most common organic solvents ^[5] , readily soluble in NG ^[5] , soluble in NG ^[3, 8] , soluble in water ^[3] , sparingly soluble in common organic solvents ^[3]
Compatibility	Storage underwater causes no loss in power ^[6]

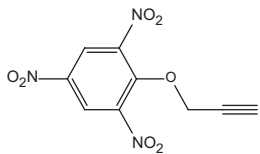
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- [10] G. Stegeman, *Heat of Combustion of Explosive Substances*, OSRD No. 5306, Division 8 National Defense Research Committee of the Office of Scientific Research and Development, USA, 4th July **1945**.

1,3,5-Trinitro-2-(prop-2-yn-1-yloxy)benzene

Name [German, acronym]: 1,3,5-Trinitro-2-(prop-2-yn-1-yloxy)benzene [PiPE]

Main (potential) use: Investigated as possible TNT replacement^[1]

Structural formula:



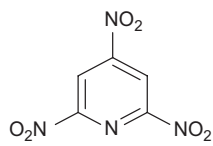
	PiPE		
Formula	C ₉ H ₅ N ₃ O ₇		
Molecular mass [g mol ⁻¹]	267.15		
Appearance at RT			
IS [J]	56.7 cm ^[1]		
FS [N]	>360 ^[1]		
ESD [J]	0.2113 ^[1]		
N [%]	15.73		
Ω(CO ₂) [%]	-80.85		
T _{m,p.} [°C]	100 ^[1]		
T _{dec.} [°C]			
ρ [g cm ⁻³]	1.612 ^[1]		
Heat of formation	227.4 (no units given) ^[1]		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
-Δ _{ex} U° [kJ kg ⁻¹]			
T _{ex} [K]			
p _{C-J} [kbar]		21.96 GPa (calcd., Cheetah 7.0) ^[1]	
VoD [m s ⁻¹]		6,929 (@ 1.612 g cm ⁻³ , calcd., Cheetah 7.0) ^[1]	
V ₀ [L kg ⁻¹]			

Vacuum stability test [cm ³ /h]	STANAG 4147 test 1B, total gas evolved after 40 h @ 100 °C, values in cc): 2.8188 ^[1]
Compatibility	VTs compatibility (STANAG 4147 test 1B, 2.5 g of compound 1 mixed with 2.5 g of compound 2, total gas evolved after 40 h @ 100 °C, values in cc) ^[1] : 1.5223 (DNGU), 1.7547 (LLM-105), – (HK-56), 1.3033 (HMX) concluding that DNGU, LLM-105, HK-56 and HMX are compatible with PiPE ^[1]

- [1] D. Price, *GrIMEx: Development of a Novel, Green IM Comp B Replacement*, Oral presentation, 2016 Insensitive Munitions and Energetic Materials Technology Symposium, Nashville, Tennessee, USA, **2016**.

Trinitropyridine

Name [German, acronym]: Trinitropyridine [trinitropyridin, TNPy]
Main (potential) use: high explosive
Structural formula:



	TNPy		
Formula	C ₅ H ₂ N ₄ O ₆		
Molecular mass [g mol ⁻¹]	214.09		
Appearance at RT	Pale yellow prism crystals ^[7] , yellow needles ^[8]		
IS [J]	4.5–6.5 Nm ^[1, 8] , 60% ^[7]		
FS [N]	>353 ^[8] , 4% ^[7]		
N [%]	26.17		
Ω(CO ₂) [%]	–37.37		
T _{m.p.} [°C]	162 (sublimation) ^[1, 8] , 164 (recryst.) ^[7] , 162–163 (endo, DTA @ 15 °C/min) ^[7] , 164.1 (endo, DSC) ^[7]		
T _{dec.} [°C]	444–445 (exo, DTA @ 15 °C/min) ^[7] , 321.5 (first exo, second exo @ 372 °C, DSC) ^[7]		
ρ [g cm ⁻³]	1.77 ^[1, 8] , 1.74 (crystal) ^[7]		
Heat of formation	368.5 kJ/kg (enthalpy of form.) ^[8]		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
–Δ _{ex} U° [kJ kg ⁻¹]			4,418 [H ₂ O (l)] ^[3, 4]
T _{ex} [K]			
p _{C-J} [kbar]			
VoD [m s ⁻¹]		7,645 ± 15 (@ 1.686 g cm ⁻³) ^[7]	7,470 (@ 1.66 g cm ⁻³) ^[8]
V ₀ [L kg ⁻¹]			818 ^[5, 8]

5 s explosion T [°C] Explosion T [°C]	Minimal T of explosion = 413 °C ^[7]												
Thermal stability	Thermal stability heated @ constant T ^[7] : <table><tr><th>T (°C)</th><th>Time (h)</th><th>Weight degression (%)</th></tr><tr><td>100</td><td>20</td><td>0.00</td></tr><tr><td>120</td><td>48</td><td>0.85</td></tr><tr><td>120</td><td>120</td><td>1.03</td></tr></table>	T (°C)	Time (h)	Weight degression (%)	100	20	0.00	120	48	0.85	120	120	1.03
T (°C)	Time (h)	Weight degression (%)											
100	20	0.00											
120	48	0.85											
120	120	1.03											
Solubility [g/mL]	Easily soluble in acetone, DMSO, dioxane, nitromethane, ethyl acetate, dil. nitric acid ^[7] , insoluble in benzene, 1,2-dichloroethane, Et ₂ O ^[7]												
Compatibility	Stable to hydrochloric acid and water ^[7]												
ΔH_{sub} [kJ/mol]	101.7 (exptl.) ^[6] , 108.7 (calcd., QSPR) ^[6]												

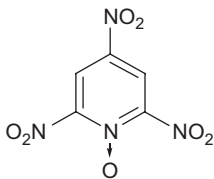
	TNPy ^[2]
Chemical formula	C ₅ H ₂ N ₄ O ₆
Molecular weight [g mol ⁻¹]	214.11
Crystal system	Orthorhombic
Space group	<i>Pbcn</i>
a [Å]	28.573(6)
b [Å]	9.7394(19)
c [Å]	8.7566(18)
α [°]	90
β [°]	90
γ [°]	90
V [Å ³]	2,436.8(8)
Z	12
ρ_{calc} [g cm ⁻³]	1.751
T [K]	293(2)

- [1] H. H. Licht, H. Ritter, *Propellants, Explosives, Pyrotechnics*, **1988**, *13*, 25–29.
- [2] J.-R. Li, J.-M. Zhao, H.-S. Dong, *J. Chem. Crystallogr.*, **2005**, *35*, 943–948.
- [3] L. R. Rothstein, R. Petersen, *Propellants, Explosives, Pyrotechnics*, **1979**, *4*, 56–60.
- [4] M. H. Keshavarz, *Propellants, Explosives, Pyrotechnics*, **2008**, *33*, 448–453.
- [5] M. Jafari, M. Kamalvand, M. H. Keshavarz, A. Zamani, H. Fazeli, *Indian J. Engineering and Mater. Sci.*, **2015**, *22*, 701–706.
- [6] H. W. Lee, K.-H. Chung, S. G. Cho, B.-S. Lee, C. K. Kim, *Predictive Studies on Various Physicochemical Properties of Explosive Molecules*, ICT **2006**, Karlsruhe, Germany, pp. 177-1–177-12.
- [7] W. Daozheng, *Chinese Sci. Bull. (Kexue Tongbao)*, **1986**, *31*, 1034–1037.
- [8] R. Meyer, J. Köhler, A. Homburg, *Explosives*, 7th edn., Wiley-VCH, Weinheim, **2016**, p. 366.

Trinitropyridine-*N*-oxide

Name [German, acronym]: Tripyridine-*N*-oxide [trinitropyridin-*N*-oxid, TNPyOX]
Main (potential) use: Used as intermediate in the production of trinitropyridine^[7]

Structural formula:



	TNPyOx		
Formula	C ₅ H ₂ N ₄ O ₇		
Molecular mass [g mol ⁻¹]	230.09		
Appearance at RT	yellow crystals ^[7]		
IS [J]	1.5–3.0 Nm ^[1, 7] , <i>H</i> ₅₀ = 20 cm ^[6, 8]		
FS [N]	157 ^[7]		
<i>N</i> [%]	24.35		
Ω(CO ₂) [%]	–27.82		
<i>T</i> _{m.p.} [°C]	170 (dec.) ^[7]		
<i>T</i> _{dec.} [°C]	170 ^[1]		
ρ [g cm ⁻³]	1.86 ^[1, 7] , 1.875 ^[8]		
Heat of formation	98.7 kJ/mol (Δ _f <i>H</i>) ^[4] , 428.9 kJ/kg (enthalpy of form.) ^[7] , 24.40 kcal/mol (Δ _f <i>H</i> (s)) ^[8] , 98.6 kJ/mol (enthalpy of form., exptl.) ^[10] , 16.8 kJ/mol (enthalpy of form., calcd., emp.) ^[10] , –18.5 kJ/mol (enthalpy of form., calcd., S-D method) ^[10] , 102.10 ± 1.30 kJ/mol (Δ _f <i>H</i> ^o _{solid}) ^[11]		
Heat of combustion	–2,355.60 ± 1.30 kJ/mol (Δ _c <i>H</i> ^o _{solid}) ^[11]		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
–Δ _{ex} <i>U</i> ^o [kJ kg ⁻¹]	5,912	1.58 kcal/g (<i>Q</i> _{max} , calcd.) ^[8]	3,533 [H ₂ O (l)] ^[4] 5,320 [H ₂ O (l)] ^[7]

T_{ex} [K]	4,298		
$p_{\text{C-I}}$ [kbar]	337	333 (@ 1.875 g cm ⁻³ , calcd.) ^[8]	
VoD [m s ⁻¹]	8,615 (@ 1.875 g cm ⁻³ , $\Delta_f H = 98.7$ kJ mol ⁻¹)	8,560 (@ 1.875 g cm ⁻³ , calcd.) ^[8] 8,369 (@ TMD, R-P method) ^[3]	7,770 (1.72 g cm ⁻³) ^[7]
V_0 [L kg ⁻¹]	667		777 ^[5, 7]

ΔH_{sub} [kJ/mol]	106.3 (exptl.) ^[9] , 108.7 (calcd., QSPR) ^[9] , 106.30 ± 2.90 @ 390 K ^[11]
$\log P_{\text{octanol/water}}$	0.04 ^[11]

	TNPY^[2]
Chemical formula	C ₅ H ₂ N ₄ O ₇
Molecular weight [g mol ⁻¹]	299.99
Crystal system	Orthorhombic
Space group	<i>Pnma</i>
a [Å]	9.6272(19)
b [Å]	14.128(3)
c [Å]	5.9943(12)
α [°]	90
β [°]	90
γ [°]	90
V [Å ³]	815.3(3)
Z	4
ρ_{calc} [g cm ⁻³]	1.875
T [K]	293

[1] H. H. Licht, H. Ritter, *Propellants, Explosives, Pyrotechnics*, **1988**, 13, 25–29.

[2] J.-R. Li, J.-M. Zhao, H.-S. Dong, *J. Chem. Crystallogr.*, **2005**, 35, 943–948.

[3] L. R. Rothstein, R. Petersen, *Propellants, Explosives, Pyrotechnics*, **1979**, 4, 56–60.

[4] M. H. Keshavarz, *Propellants, Explosives, Pyrotechnics*, **2008**, 33, 448–453.

[5] M. Jafari, M. Kamalvand, M. H. Keshavarz, A. Zamani, H. Fazeli, *Indian J. Engineering and Mater. Sci.*, **2015**, 22, 701–706.

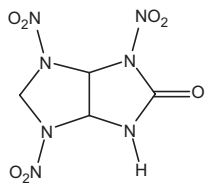
- [6] C. B. Storm, J. R. Stine, J. F. Kramer, *Sensitivity Relationships in Energetic Materials*, NATO Advanced Study Institute on Chemistry and Physics of Molecular Processes in Energetic Materials, LA-UR-89-2936, **1990**.
- [7] R. Meyer, J. Köhler, A. Homburg, *Explosives*, 7th edn., Wiley-VCH, Weinheim, **2016**, p. 366.
- [8] P. Politzer, J. S. Murray, *High-Performance, Low Sensitivity: The Impossible (or Possible) Dream?* in *Energetic Materials From Cradle to Grave*, M. K. Shukla, V. M. Boddu, J. A. Steevens, R. Damavarapu, J. Leszczynski (eds.), Springer Verlag, **2017**, pp. 1–22.
- [9] H. W. Lee, K.-H. Chung, S. G. Cho, B.-S. Lee, C. K. Kim, *Predictive Studies on Various Physicochemical Properties of Explosive Molecules*, ICT **2006**, Karlsruhe, Germany, pp. 177-1–177-12.
- [10] B. Nazari, M. H. Keshavarz, M. Hamadani, S. Mosavi, A. R. Ghaedsharafi, H. R. Pouretedal, *Fluid Phase Equilibria*, **2016**, 408, 248–258.
- [11] 2,4,6-Trinitropyridine 1-oxide Datasheet: <https://www.chemeo.com/cid/33-744-9/2%2C4%2C6-Trinitropyridine%201-oxide>

2,4,6-Trinitro-2,4,6,8-tetraazabicyclo[3.3.0]-octane-3-one

Name [German, acronym]: 2,4,6-Trinitro-2,4,6,8-tetraazabicyclo[3.3.0]-octane-3-one
[HK-55]

Main (potential) use: high explosive

Structural formula:



	HK-55			
Formula	C ₄ H ₅ N ₇ O ₇			
Molecular mass [g mol ⁻¹]	263.13			
Appearance at RT	White powder ^[3] , white microcrystals (recryst. from CH ₃ CN) ^[3]			
IS [J]	DH ₅₀ = 61 cm ^[1] , 61 cm (cf. 32 cm for HMX) ^[3]			
	Data from ^[2] :			
	% purity	Holston impact (cm)	% purity	Holston impact (cm)
	~99.5	~ 25	99.4	~ 20
	99.2	~ 20–25	95.8	~ 20–25
	99.7	~ 20	~ 98–99	~ 20–25
	98.9	~ 20–25	~ 98–99	~ 15–20
N [%]	37.26			
Ω(CO ₂) [%]	–21.28			
T _{m,p.} [°C]	196 ^[1] , 196–197 ^[3]			
T _{dec.} [°C]				
ρ [g cm ⁻³]	1.905 ^[1, 3]			
Heat of formation				

	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^\circ$ [kJ kg ⁻¹]			
T_{ex} [K]			
p_{CJ} [kbar]			
VoD [m s ⁻¹]			
V_0 [L kg ⁻¹]			
Solubility [g/mL]	Recryst. from CH ₃ CN ^[3]		

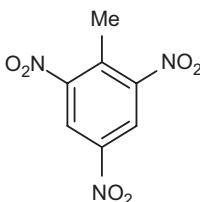
- [1] P. F. Pagoria, G. S. Lee, A. R. Mitchell, R. D. Schmidt, *Thermochim. Acta*, **2002**, 384, 187–204.
 [2] D. Price, J. Morris, S. Haedrick, N. Tucker, R. Uy, *Energetic Ingredients Synthesis*, BAE systems presentation, Holston Army Ammunition Plant, October **2013**.
 [3] P. F. Pagoria, A. R. Mitchell, E. S. Jessop, *Propellants, Explosives, Pyrotechnics*, **1996**, 21, 14–18.

2,4,6-Trinitrotoluene

Name [German, acronym]: 2,4,6-Trinitrotoluene, 1,3,5-trinitro-2-methylbenzene, tritol, triton, tritone, trotol, trilita, trotyl [2,4,6-trinitrotoluol, trinitrotoluol, tri, trotyl, tutol, trinol, Füllpulver 1902, Sprengmunition 02, TNT, Fp02][†]

Main (potential) use: Secondary (high) explosive, melt cast, demolition, compressed (in demolition charges)^[88], cast TNT in shells and demolition charges^[88], large caliber armor-piercing shells^[88]

Structural formula:



[†] Commercial TNT for military purposes is the 2,4,6-TNT isomer (α -TNT)^[88]; there are different standards in different countries for different grades of TNT^[88]. Crude TNT (de Beule) has the following composition: 95.1% α -TNT, 1.36% β -TNT, 2.69% γ -TNT, 0.002% δ -TNT, 0.009% ζ -TNT and dinitrotoluene isomers by nitration of *m*-nitrotoluene^[88]; Values below given for α -TNT (2,4,6-TNT) unless otherwise indicated

	2,4,6-TNT
Formula	C ₇ H ₅ N ₃ O ₆
Molecular mass [g mol ⁻¹]	227.13
Appearance at RT	Light yellow solid ^[23] , yellow, crystalline solid ^[27] , crystallizes as small columns or needles ^[88] , all isomers (α -, β -, γ -, δ -, ζ -) are pale yellow crystalline solids ^[88] , straw yellow–yellow-brown flaked, granular or crystalline material – color depends on purity ^[142] , colorless or light yellow rhombohedral crystals (α -TNT) ^[149] , white substance which becomes yellow in light and has two polymorphic forms ^[163]
IS [J]	15 Nm ^[1, 8] , 39.24 ^[6] , 35.86 (first reaction) ^[13, 106] , 39.24 (sound) ^[13, 106] , 18.64–19.62 (95–100 + cm, 2 kg mass, 20 mg sample, B. M.) ^[17, 18, 23] , 6.98–7.48 (14–15 in, 2 kg mass, 17 mg sample, P. A.) ^[17, 18, 23, 165] , IS _{LL} = 5.0 m ^[26] , IS _{A50} = 6.5 m ^[26] , H ₅₀ = 212 cm (tool type 12, flake TNT) ^[25] , H ₅₀ > 320 cm (tool type 12B, flake TNT) ^[25] , H ₅₀ = 154 cm (tool type 12, granular TNT) ^[25] , H ₅₀ > 320 cm (tool type 12B, granular TNT) ^[25] ,

$H_{50} > 111.6$ ^[29], $H_{50\%} = 200$ cm (US NOL app.)^[28], $H_{50\%} = 200$ cm (35 mg sample, 2.5 kg mass, US NOL app.)^[91], $H_{50\%} = 160$ cm^[46], 197 cm (media height, 5 kg mass, 30 mg sample, Rotter app.)^[44], $H_{50} = 80$ cm (tool type 12, 5 kg mass)^[51], $H_{50} \geq 177$ cm (tool type 12B, 5 kg mass)^[51], > 29.43 (Julius-Peters app.)^[53], $Ed_{\min} = 25-35$ (BAM, 5 kg mass, max. level at which six negative results obtained)^[54], $H_{50\%} = 98$ cm (B.M., type 12 tool, 2.5 kg mass, 35 mg sample, garnet paper)^[55], 88.3 cm^[73], $H_{50} = 60$ cm (5 kg hammer)^[78], $H_{50} = 160$ cm^[81], 94 cm (pressed TNT, NEDED)^[85], 210 cm (pressed TNT, NOL)^[85], 148 cm (pressed TNT, LANL)^[85], 94 cm (cast TNT, NEDED)^[85], 210 cm (cast TNT, NOL)^[85], 148 cm (cast TNT, LANL)^[85], $H_{50} > 111.6$ J^[86], molten TNT is more sensitive to impact than cryst. TNT^[88], $H_{50\%} = 160-200$ cm (TNT powder, 0.5 kg hammer)^[91], $H_{50\%} \geq 200$ cm (0.5 kg hammer)^[91], $(H_{50}W_g)^{-1} = 15$ Nm^[95], 60–180 cm (2 kg mass)^[93], $H_{50\%} = 150-215$ cm^[96], $H_{50\%} = 110$ cm (5 kg mass, several decigrams sample contained in 0.2 mm thickness small iron cup covered with iron disc of same thickness)^[93], 8.4 J/s $\times 10^{-4}$ (threshold above which initiation occurs)^[102], $H_{50\%} = 200$ cm^[104], 160 cm (Bruceton method, type 12 tool, 2.5 kg mass, 40 mg sample, 5/0 sandpaper, 25 trials)^[107], 160 cm (2.5 kg mass)^[111], 105.4 cm (2.5 kg mass, AFATL)^[111], 61.7 cm (5 kg mass, AFATL)^[111], $H_{50} = 110$ cm (2.5 kg mass, Bruceton method, NOL machine, type 12 tool, 35 \pm 2 mg sample, 5/0 sandpaper)^[127], 33.8^[128], 15 (BAM)^[130], $Ed_{\min} = 25-35$ (BAM, 5 kg mass, RT)^[131], $H_{50} = 98$ cm (2.5 kg mass, type 12 tool)^[136], $\log(H_{50}) = 2.196$ (Kamlet/Adolph)^[137], 1,570 mm (dropheight, Rotter impact test)^[139], 1,006 mm (dropheight, Rotter impact test, +5% DETA)^[139], > 100 cm (max dropheight for 0 explosions in 5 trials, 2,000 g mass, 0.02 g sample, B.M. small impact device)^[145], > 200 cm (TNT powder, 0.5 kg)^[146], $H_{50\%} = 160$ cm (2.5 kg mass, type 12 tool, ERL method)^[161], 95 cm (B.M.)^[165], 227 cm (50% point, type 12 tool, 2.5 kg mass, sandpaper)^[168], $A_{d1} = 8\%$, $A_{d2} = 0\%$, $LL = 5.0$ m, $A_{50\ d1} = 6.5$ m, $A_{50\ d2} = 14.0$ ^[176], 35.6 cm (P.A.)^[181], > 95 cm (B.M.)^[181]

P.A. apparatus (@ °C): 8.47(@ -40 °C), 6.98 (@ RT), 3.49 (@ 80 °C), 1.50 (@ 90 °C)^[23]

Large impact apparatus; pressed @ 1.60 g cm⁻³ = 34.9^[23]; cast @ 1.60 g cm⁻³ = 12.96^[23]

IS (2 kg mass, P.A. apparatus @ different temperatures)^[23, 27, 33]:

T (°C)	inches
-40	17
RT	14
80	7
90	3
105	2 (5 explosions from 20 trials)

Max. fall for $0/6$ shots >60 cm (2 kg mass, Lenze-Kast apparatus)^[30], max. fall for $0/6$ shots >24 cm (10 kg mass, Lenze-Kast apparatus)^[30], min. fall for $6/6$ shots >60 cm (2 kg mass, Lenze-Kast apparatus)^[30], min. fall for $6/6$ shots >24 cm (2 kg mass, Lenze-Kast apparatus)^[30], similar @ 90 °C to that of PA @ RT^[88], 197 cm (median height, 5 kg mass, 30 mg sample, Fol = 152 cf. RDX = 80, Rotter apparatus)^[181]

Powdered samples: $H_{50\%}$ = 157 cm (NOL app.)^[44], 154 cm (LASL app.)^[44], 183 cm (B.M. app. @ ERL)^[44], $H_{10\%}$ = 98 cm (B.M. app. @ P.A.)^[44], $H_{10\%}$ = 15 in (P.A.)^[44]

Max. no-fire height in cm, 2 kg mass, 2 mg ground samples^[101]:

Sample	Uncycled	Cycled 1 × to 150 °C @ 5 °C/min	Cycled 2 × to 150 °C @ 5 °C/min	Ambient –200 °C @ 40 °C/min, hold for 30 min.
Virgin TNT	42	58	56	84
	42	52	64	60
Reclaimed flake TNT	50	58	54	–
	52	64	60	–

Piston apparatus, 100 trials per height^[88]:

$T(^{\circ}\text{C})$	% Explosions @ height (cm)		
	25 cm	30 cm	50 cm
18	–	24	54
20	11	–	–
80	13	–	–
81	–	31	59
90	–	48	75
100	25	63	89
110	43	–	–
120	62	–	–

Variation of IS with temperature^[165]:

T (°C)	50% point (in)
30	23.6
50	22.0
70	17.0
75	14.2
85	4.73
90	5.12
110	3.54
130	3.15

Rotter impact data: 27 mg sample, Bruceton method/25 drop run to obtain $H_{50\%}$; initiation criteria = 1 mL gas evolved or 0.5 mL accompanied by smoke or evidence of burning in the sample; data from^[184]:

Rotter impact data		US data	
F of I	Gas evolved (mL)	NSWC/NOL, ERL type 12	NWC B.M. type 12
150–200	2,157	157	74, 98

FS [N]

353^[1, 8], unaffected by steel shoe (friction pendulum test)^[23, 165], unaffected by fiber shoe (friction pendulum test)^[23], unaffected by pendulum friction test^[27, 149], $P_{fr,LL} = 600$ MPa^[26, 176], $P_{fr,50\%} = 850$ MPa^[26, 176], $F_{50} = 8$ (1/6) kgf^[29], mean FOF (figure of friction) >8.2 (Rotter FS)^[36], >360 (mean limiting load, BAM)^[36], $G_{min} \geq 360$ (Julius-Peters, max. level at which six negative results obtained)^[54], 168^[73], 50% value ≥ 360 (BAM)^[76], $F_{50} = 8$ kgf (1/6)^[86], very low, but is higher when TNT is molten^[88], Rotter FoF = 5.8^[92], Rotter FOF = 6^[92], 360 (BAM, limiting load)^[92], 36 KPa $\times 10^{-4}$ @ 2.4 m/s (threshold above which initiation occurs)^[102], 1,100^[128], 10% go @ 353 (Julius Peter apparatus)^[130], $G_{min} \geq 360$ (BAM Julius Peters, max level with six consec. negative runs)^[131], unaffected by Picatinny Arsenal friction test^[181]

Torpedo friction = 80–120 cm (1 kg @ 80 °C, 0.5 m/s)^[91, 146], Torpedo friction = 100–120 cm (TNT powder, 1 kg @ 80 °C, 0.5 m/s)^[91], friction wheel ≥ 50 kg (1 kg @ 80 °C, 0.5 m/s)^[91, 146]

Mallet friction test: steel on steel = 0%^[36], nylon on steel = 0%^[36], wood on softwood = 0%^[36, 171], wood on hardwood = 0%^[36, 171], wood on Yorkstone = 0%^[36, 171]

ESD [J]

6.85^[6, 9, 12], 111.8 mJ^[9], 0.06 (100 mesh, unconfined)^[23, 48], 4.4 (100 mesh, unconfined)^[23, 48], spark sensitivity = 0.46 (brass electrode, 3 mil Pb foil thickness)^[25], 2.75 (brass electrode, 10 mil Pb foil thickness)^[25], 0.19 (steel electrode, 1 mil Pb foil thickness)^[25], 4.00 (steel electrode, 10 mil Pb foil thickness)^[25], 0.06 (unconfined, 100 mesh)^[27], 4.4 (confined, 100 mesh)^[27], $E_{50}=8.576$ (@ 293 K)^[29], $E_{50}=5.470$ (@ 333 K)^[29], $E_{50\%}=8.576$ ($T_0=293$ K)^[86], $E_{50\%}=5.470$ ($T_0=333$ K)^[86], $E_{50\%}=0.57\pm0.13$ (Bruceton equation)^[94], >156 mJ (closed container)^[121], >156 mJ (open container)^[121], 0.46 (Nexter Munitions apparatus)^[130], 0.06 (unconfined)^[165], 0.44 (confined)^[165], 0.036 (12,000 V, 100 sieve, for zero ignition, 500 MMF capacitance, 0.005 in gap setting)^[178], 0.06 (static electricity, unconfined)^[181], 0.44 (static electricity, confined)^[181]

Highest energy (J) for zero ignition probability^[178]:

Results from ^[178]	Bureau of Mines, 1943	Bureau of Mines, 1946
0.036	0.077	0.062

Highest electrostatic discharge energy (J) @ 5,000 V for zero ignition probability^[31]:

	Highest E (J) for zero ignition probability		Type of ignition	
	Unconfined	Confined	Unconfined	Confined
TNT granular	> 11.0	4.68	None	Deton.
TNT granular through 100 mesh	0.062	4.38	Deflag.	Deton.

Data from^[180]:

Material	50% point energy (J)		
	3-mil foil	10-mil foil	% expl.
TNT (Impact Std)	0.46	3.75	0

	Mallet FS, % ignitions ^[181] : <table><tr><th colspan="3">Mild steel mallet on anvils of</th><th colspan="3">Standard wood mallet on anvils of</th></tr><tr><th>Mild steel</th><th>Naval brass</th><th>Aluminum bronze</th><th>York stone</th><th>Hardwood</th><th>Softwood</th></tr><tr><td>0</td><td>0</td><td>0</td><td>0</td><td>0</td><td>0</td></tr></table> <p>Pendulum FS: passed fiber shoe^[181], passed steel shoe^[181]</p>	Mild steel mallet on anvils of			Standard wood mallet on anvils of			Mild steel	Naval brass	Aluminum bronze	York stone	Hardwood	Softwood	0	0	0	0	0	0
Mild steel mallet on anvils of			Standard wood mallet on anvils of																
Mild steel	Naval brass	Aluminum bronze	York stone	Hardwood	Softwood														
0	0	0	0	0	0														
N [%]	18.5																		
Ω(CO ₂) [%]	−74.0																		
T _{phase transitions} [°C]	<p>No reversible phase transitions in contrast to observations from calorimetric measurements^[41], calorimetric measurements suggests orthorhombic TNT undergoes phase transformation possibly to monoclinic form @ 343 K^[156], monoclinic TNT stable from ambient temperature until mpt.^[156], monoclinic→ orthorhombic transformation occurs @ ambient temperature over long periods of time^[156]</p> <p>~70 (small endo, orthorhombic → monoclinic, DSC @ 1–10 K/min (followed by endo @ 81 °C corresponding to monoclinic mpt.))^[41]</p> <p>354 K (small peak, orthorhombic)^[35], orthorhombic is stable under ambient conditions and transforms to monoclinic over time^[177], orthorhombic → monoclinic transformation is instantaneous @ 344 K^[177], monoclinic form is stable up to mpt. of 354 K^[177]</p>																		
T _{glass transition} [°C]	−15 (glass is metastable <−15°C, formed by very rapid quenching of molten TNT @ 64 °C/min) ^[35] , −14 – −8 (glass transforms to crystalline solid) ^[35]																		
T _{m.p.} [°C]	81 ^[23, 33, 96, 104] , 80–82 ^[21] , 80.9 ^{[25], [33]} , 80.6 ^[30, 130] , 80.6–80.85 ^[33] , 80.75 ± 0.05 ^[33] , 81.5 ^[33] , 81.5 (annealed TNT, DTA @ 10 °C/min) ^[34] , 79.5–80.5 (melt-quenched TNT, DTA @ 10 °C/min) ^[34] , 81 (endo, monoclinic TNT, DSC @ 1–10 K/min) ^[41] , 80 ^[47, 73, 76, 120] , 80.7 ^[48, 171] , 80.8 ^{[48], [109]} , 75–100 (endo, 20 mg sample, DTA @ 10 °C/min) ^[33] , 355 K (monoclinic, DSC) ^[35] , 354 K (mpt. of sample after orthorhombic converted to monoclinic) ^[35] , 80.1–81.6 ^[77] , 81.6 (DSC, sample in sealed cell) ^[86] , various values reported: 80.6, 80.65, 80.0 80.85, 80.66 ^[88] , 112 (β-TNT, 2,3,4-TNT) ^[93] , 104 (γ-TNT, 2,4,5-TNT) ^[93] , 79.5 (ζ-TNT, 2,3,6-TNT, only trace quantities of this isomer have been synthesized) ^[93] , 80.66 (DSC, 5 mg sample, Al pan, Al cover without crimping, 5 °C/min, under N ₂ flow, mean value of 7 measurements with a standard deviation of 0.099) ^[97] , 80.7 (Thomas Hoover Capillary Melting Point Apparatus @ 2 °C/min) ^[109] , 79.93 (endo, onset, DSC @ 10 °C/min, 1–10 mg sample, unsealed but covered Al pans) ^[112] , 80.63																		

	<p>(endo, onset, 92.12 J/g, DSC @ 10 °C/min, 1–10 mg sample, unsealed but covered Al pans)^[112], 80.75^[138, 149], 80–81^[27, 142], 80.1^[152], no dec. on melting with no dec. observed on melting and solidifying >60 times^[27], 345 K (monoclinic crystal)^[156], 81 (cast)^[165], 79 (uncycled) and 78 (cycled TNT)^[167]</p> <p>79 (TGA/DTA, 10 mg sample, in air, open Al pans)^[99]</p> <p>Effect of prolonged heating on mpt.^[88]:</p> <table><tr><th>Conditions before mpt. measured</th><th>mpt. (°C)</th><th>Conditions before mpt. measured</th><th>mpt. (°C)</th></tr><tr><td>18 h heating @ 145–150 °C</td><td>80.66</td><td>127 h heating @ 145–150 °C</td><td>80.20</td></tr><tr><td>42 h heating @ 145–150°</td><td>80.55</td><td>158 h heating @ 145–150 °C</td><td>80.13</td></tr><tr><td>80 h heating @ 145–150 °C</td><td>80.25</td><td>177 h heating @ 145–150 °C</td><td>79.90</td></tr></table> <p>Effect of prolonged heating on mpt.^[88]: mpt. = 78 °C (after heating @ 180 °C for 290 min)^[88], mpt. = 17 °C (after heating @ 201 °C for 180 min)^[88], mpt. = 59 °C (after heating @ 217.5 °C for 45 min)^[88]</p> <p>mpt. decreases from 80.0 to 79.5 °C after 2 weeks sunlight irradiation (<i>Kast</i>)^[88], mpt. decreases from 80 to 74 °C after exposure to sunlight in the open for 3 months^[88], TNT irradiated in absence of air in vacuum showed no change in mpt.^[88]</p> <p>112 (β-TNT, 2,3,4-TNT)^[88], 104 (γ-TNT, 2,4,5-TNT)^[88], 137 (δ-TNT, 3,4,5-TNT)^[88], 97.5 (ε-TNT, 2,3,5-TNT)^[88], 111 (ζ-TNT, 2,3,6-TNT)^[88]</p>	Conditions before mpt. measured	mpt. (°C)	Conditions before mpt. measured	mpt. (°C)	18 h heating @ 145–150 °C	80.66	127 h heating @ 145–150 °C	80.20	42 h heating @ 145–150°	80.55	158 h heating @ 145–150 °C	80.13	80 h heating @ 145–150 °C	80.25	177 h heating @ 145–150 °C	79.90
Conditions before mpt. measured	mpt. (°C)	Conditions before mpt. measured	mpt. (°C)														
18 h heating @ 145–150 °C	80.66	127 h heating @ 145–150 °C	80.20														
42 h heating @ 145–150°	80.55	158 h heating @ 145–150 °C	80.13														
80 h heating @ 145–150 °C	80.25	177 h heating @ 145–150 °C	79.90														
$T_{\text{freezing point}}$ [°C]	<p>80^[163], 85^[163]</p> <p>Effect of moisture on freezing point of TNT^[27]:</p> <table><tr><th>% Water</th><th>Freezing point (°C)</th></tr><tr><td>0</td><td>80.59</td></tr><tr><td>0.1</td><td>80.35</td></tr><tr><td>0.2</td><td>80.20</td></tr><tr><td>0.3</td><td>79.99</td></tr><tr><td>0.5</td><td>79.78</td></tr><tr><td>1.0</td><td>79.09</td></tr><tr><td>2.5</td><td>77.93</td></tr></table>	% Water	Freezing point (°C)	0	80.59	0.1	80.35	0.2	80.20	0.3	79.99	0.5	79.78	1.0	79.09	2.5	77.93
% Water	Freezing point (°C)																
0	80.59																
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0.2	80.20																
0.3	79.99																
0.5	79.78																
1.0	79.09																
2.5	77.93																

	<p>Removal of moisture from TNT; effect of moisture on freezing point, water content = 0.3% before drying^[27]:</p> <table> <tr> <th>Hours of heating at 100 °C</th><th>freezing point of sample (°C)</th></tr> <tr> <td>0</td><td>79.99</td></tr> <tr> <td>2</td><td>80.30</td></tr> <tr> <td>3.5</td><td>80.46</td></tr> <tr> <td>5</td><td>80.55</td></tr> <tr> <td>6</td><td>80.59</td></tr> </table>	Hours of heating at 100 °C	freezing point of sample (°C)	0	79.99	2	80.30	3.5	80.46	5	80.55	6	80.59
Hours of heating at 100 °C	freezing point of sample (°C)												
0	79.99												
2	80.30												
3.5	80.46												
5	80.55												
6	80.59												
$T_{b.p.}$ [°C]	<p>240 (explodes)^[77], can be distilled off @ 210–212 @ 10–12 mm Hg without visible dec.^[88], 190 @ 2 mm Hg^[88, 89], 245–250 @ 50 mm Hg^[88, 89], extrapolated value @ normal pressure = 300 ± 10 °C^[88, 89], direct determination of bpt. not possible since it is close to the initiation temperature of TNT^[88], 345 (@ 760 mm Hg, condensation T of TNT vapors)^[88], 232 (@ 30 mm Hg, condensation T of TNT vapors)^[88], 210–212 @ 10–20 mm Hg^[93], 345 (@ atmospheric pressure)^[27], 190 (@ 2 Torr)^[27], 210 (@ 10–12 Torr)^[27], 245–250 °C (@ 50 Torr)^[27]</p>												
$T_{dec.}$ [°C]	<p>290 (DSC @ 5 °C/min), 526 K (DTA)^[13, 106], 260–310 (exo, 20 mg sample, DTA @ 10 °C/min)^[33], 328 (exo peak max., DSC @ 20 °C/min)^[47], 190 (TG onset)^[76], 250–300 (exo peak, DSC, 5 mg sample, Al pan, Al cover without crimping, 5 °C/min, under N₂ flow)^[97], 274.47 (exo, onset, DSC @ 10 °C/min, 1–10 mg sample, unsealed but covered Al pans)^[112], 209 (ARC, heat-wait-search procedure, T raised from RT to 100 °C then from 100 °C onward in 5 °C steps, at each step system was maintained adiabatic, exotherm was defined as a self-heating rate exceeding 0.02 °C/min, Ar atmosphere)^[117], 294.8 (exo peak, DTA)^[124], 225 (deflagration T, determined using 2 lb slabs heated @ 100 °C/min on one surface)^[96]</p> <p>TGA/DTA (10 mg sample, in air, open Al pans): 125 (start of mass loss), 161 (3% mass loss), 180 (endothermic sublimation)^[99]</p> <p>DSC (closed Al pans, 1 K/min): 315.3 (exo peak onset), 324.0 (exo peak max)^[99]</p> <p>@ 8 °C/min: $T_{idb} = 269.4$, $T_w = 279.3$, $T_{max} = 282.9$^[56]</p> <p>@ 16 °C/min: $T_{idb} = 309.1$, $T_w = 318.3$, $T_{max} = 323.1$^[56]</p> <p>$T_{cr} = 287$–289^[56]</p>												

	Thermal dec. induction periods (s) ^[101] :																																			
	<table><tr><th>Sample</th><th>@ 255 °C</th><th>@ 260 °C</th><th>@ 265 °C</th><th>@ 270 °C</th><th>@ 275 °C</th><th>@ 280 °C</th></tr><tr><td>Flake, uncycled</td><td>725</td><td>526</td><td>469</td><td>394</td><td>344</td><td>300</td></tr><tr><td>Flake TNT cycled 1x @ 150 °C @ 5 °C/min</td><td>537</td><td>488</td><td>444</td><td>412</td><td>313</td><td>281</td></tr><tr><td>Flake TNT cycled 2x @ 150 °C @ 5 °C/min</td><td>785</td><td>463</td><td>382</td><td>288</td><td>250</td><td>213</td></tr><tr><td>Flake TNT held @ 200 °C for 20 min</td><td>719</td><td>513</td><td>375</td><td>388</td><td>269</td><td>256</td></tr></table>	Sample	@ 255 °C	@ 260 °C	@ 265 °C	@ 270 °C	@ 275 °C	@ 280 °C	Flake, uncycled	725	526	469	394	344	300	Flake TNT cycled 1x @ 150 °C @ 5 °C/min	537	488	444	412	313	281	Flake TNT cycled 2x @ 150 °C @ 5 °C/min	785	463	382	288	250	213	Flake TNT held @ 200 °C for 20 min	719	513	375	388	269	256
Sample	@ 255 °C	@ 260 °C	@ 265 °C	@ 270 °C	@ 275 °C	@ 280 °C																														
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Flake TNT held @ 200 °C for 20 min	719	513	375	388	269	256																														
ρ [g cm ⁻³]	<p>1.713 (@ 100 K), 1.47 (molten)^[1], 1.648 (@ 298 K), 1.65 (crystal)^[23, 44, 165], 1.652, 1.653^[21], 1.654 (@ 25 °C)^[30], 1.654 (crystal, by flotation)^[33], 1.648 (cast, gas comparison pycnometer technique)^[33], 1.654 (@ TMD)^[33, 153], up to 1.64 (pressed)^[33], 1.59 (cast)^[44], 1.654^[81], 1.65 (TMD)^[86], 1.54–1.62 (compressed under pressure varying from 1,450 to 4,350 kg/cm²)^[88], 1.62 (pressed TNT, 97.5% TMD, loading pressure = 10,000 psi (75 °C))^[96], 1.651 (cast TNT, TMD)^[96], 1.619 (cast TNT, exptl. value, 98.1% TMD)^[96], 1.651 (crystal)^[104], 1.619 (exptl. ρ)^[104], 1.65^[138, 171], 1.654 (crystal)^[27, 149], 1.56 (cast)^[149], 1.55 (pressed @ 20,000 psi)^[149], 1.5–1.6 (cast)^[27], 1.63–1.64 (max. pressed)^[27], sp. gr. = 1.663^[163], sp. gr. = 1.467 (fuzed material @ 82 °C)^[163], gravimetric density = 0.9–1.0 (crystalline)^[163], 1.54 (pressed @ 1,450 kg/cm²)^[163], 1.60 (pressed @ 4,350 kg/cm²)^[163], 1.55–1.60 (cast TNT obtained on rapid cooling and agitation of fuzed α-TNT)^[163], 1.59 (cast)^[165]</p> <p>Density (g/cc) values from^[23]:</p> <table><tr><th>°C</th><th>State</th><th>g/cc</th></tr><tr><td>27–70</td><td>Flaked</td><td>1.65</td></tr><tr><td>80</td><td>Flaked</td><td>1.64</td></tr><tr><td>82</td><td>Liquid</td><td>1.48</td></tr><tr><td>87</td><td>Liquid</td><td>1.48</td></tr><tr><td>95</td><td>Liquid</td><td>1.47</td></tr></table>	°C	State	g/cc	27–70	Flaked	1.65	80	Flaked	1.64	82	Liquid	1.48	87	Liquid	1.48	95	Liquid	1.47																	
°C	State	g/cc																																		
27–70	Flaked	1.65																																		
80	Flaked	1.64																																		
82	Liquid	1.48																																		
87	Liquid	1.48																																		
95	Liquid	1.47																																		

ρ of air saturated TNT^[33]: 1.4718 @ 72.3 °C^[33], 1.4652 @ 79.2 °C^[33], 1.4588 @ 86.2 °C^[33], 1.4538 @ 92.4 °C^[33]

Pressure (kpsi)	Loading ρ (g cm ⁻³)
3	1.34 ^[27, 44, 165]
5	1.40 ^[27, 44, 165]
10	1.47 ^[27, 44, 165]
12	1.49 ^[27, 44, 165]
15	1.52 ^[27, 44, 165]
20	1.55 ^[27, 44, 165]

Loading density (g/cc), cast = 1.58–1.59, pressed psi $\times 10^{3[23]}$:

Pressure (psi $\times 10^3$)	3	5	10	15	20	30	50
ρ (g cm ⁻³)	1.35	1.40	1.45	1.52	1.55	1.59	1.6

Average densities of loading depending on the pressure applied^[88]:

Pressure applied (kg/cm ²)	ρ (g cm ⁻³)	Pressure applied (kg/cm ²)	ρ (g cm ⁻³)
215	1.320	2,750	1.599
685	1.456	3,435	1.602
1375	1.558	4,125	1.610
2,000	1.584		

Solidifying molten TNT under pressure^[88]:

Pressure (kg/cm ²)	Mean ρ (g cm ⁻³)	Pressure (kg/cm ²)	Mean ρ (g cm ⁻³)
1	1.54	4	1.616
2	1.58	5	1.620
3	1.60		

sp. gr. = 1.654–1.663 (crystals)^[88], sp. gr. = 1.467 (molten product @ 82 °C)^[88], sp. gr. = 1.57 (α -TNT allowed to slowly solidify after being melted)^[88], sp. gr. = 1.59–1.61 (α -TNT rapidly cooling with stirring from being molten)^[88]

Density of solid and liquid TNT at various temperatures^[162]:

Temperature (°C)	Specific gravity	Specific volume	Aggregate condition
25	1.6407	0.6095	Solid
40	1.6369	0.6109	Solid
50	1.6318	0.6128	Solid
55	1.6305	0.6133	Solid
60	1.6299	0.6135	Solid
65	1.6274	0.6145	Solid
70	1.6242	0.6157	Solid
72	1.6151	0.6192	Solid
75	1.5671	0.6381	Solid
78	1.5149	0.6601	Solid
79.5	1.4982	0.6672	Solid
81	1.4638	0.6832	Liquid
82	1.4634	0.6833	Liquid
88	1.4584	0.6857	Liquid
93	1.4516	0.6889	Liquid

Values from^[25]:

Method of determination	State	T (°C)	Density (g/cm ³)	
			Monoclinic	Orthorhombic
X-ray data	Solid	21	1.653	1.646
Direct measurement	Solid	21	1.654	-
Direct measurement	Liquid	83–120	1.545–1.016 × 10 ⁻³ T (°C)	

Pressed charges, compression without application of vacuum to remove residual air^[25]:

Pressure (psi)	Density (g/cm ³)
3,000	1.35
5,000	1.40
10,000	1.45
15,000	1.52
20,000	1.55
50,000	1.60

1.63–1.64 @ 20,000 psi pressure, @ 70 °C powder temperature
(compaction with residual air removed and TNT preheated to 70 °C)^[25]

Cast charges, ρ varies depending on melt, cast and solidifying procedures;
open melt = TNT melted at atmospheric conditions; vacuum melt = molten
TNT subjected to vacuum of ~ 20 mm Hg for a few minutes^[25]:

Preparative procedure			Density (g/cm ³)
Melting	Casting	Solidification	
Open	100% liquid	Ambient	1.56–1.59
Open	75% liquid	Ambient	1.59–1.61
Vacuum	50–75% liquid	Ambient	1.61–1.62

Heat of formation

–17.8 kcal mol^{–1}^[74], –15.1 kcal/mol (ΔH_f (s))^[81], –75.3 kJ mol^{–1} (ΔH_f)^[82],
–74.52 kJ/mol^[153], –295.3 kJ/kg (enthalpy of form.)^[1], –295.3 kJ/mol
(ICT thermochemical database)^[105], –48 cal/g^[7], 79 cal/g^[7], 78.5 kcal/kg^[23, 28],
–37.81 kcal/mol^[104], 44.6 kcal/kg (heat of form. (Q))^[162], –63.0 kcal/g
(enthalpy of form.)^[108], –15.1 kcal/mol (ΔH_f° , liq. or crystal)^[33], –19.25
± 0.74 kcal/mol (ΔH_f°)^[33], 16.03 ± 0.65 kcal/mol (ΔH_f°)^[33], –70.5 kcal/kg
(ΔH_f)^[86], –1.76 kcal/mol (ΔH_f° , gas)^[33], 50.92 ± 0.83 kcal/mol (ΔG_f° , free
energy of formation for crystal)^[33], 17.81 kcal/mol (– ΔH_f (heat of form. @
standard conditions))^[185], –12.0 kcal/mol (ΔH°)^[25], 29.1 kcal/mol (calcd. from
measured heat of combustion, assuming C_{amorph})^[88], 128.2 kcal/kg
(for C_{diamond})^[88], 10.2 kcal/mol (for C_{diamond})^[88], 16.0 kcal/mol (Kas)^[88],
7.7 kcal/mol (Bichel)^[88], 5.9 kcal/mol (Koehler)^[88], –17.82 kcal/mol^[96],
10–19.99 kcal/mol (heat of formation for liquid or crystal)^[27]
Heat of formation (for amorphous C): 16.0 kcal/mol (β -TNT)^[88], 24.2 kcal/mol
(γ -TNT)^[88], 21.7 kcal/mol (δ -TNT)^[88], 26.0 kcal/mol (ϵ -TNT)^[88], 24.5 kcal/mol
(η -TNT)^[88]

Heat of combustion	<p>3,620 kcal/kg^[23, 28], 822.5 cal/mol (@ C^v, exptl. value, calorimetric bomb)^[88], $-\Delta H_c$ (crystal) = 809.90 kcal/mol^[33], $-\Delta H_c$ (crystal) = 817.2 kcal/mol^[33], ΔH_c = 14,080 kJ/kg^[76], heat of combustion for the crystal = 809.18– 817.2 kcal/mol^[27], heat of combustion = 3,620 cal/g (cast TNT)^[165], Heat of combustion (@ C^v with correction for nitric acid): 834.1 kcal/mol (β-TNT)^[88], 827.4 kcal/mol (γ-TNT)^[88], 829.9 kcal/mol (δ-TNT)^[88], 825.6 kcal/ mol (ϵ-TNT)^[88], 827.1 kcal/mol (η-TNT)^[88], 3,596 kcal/kg @ C^v^[162], ΔH_c° = –817.2 kcal/mol^[25]</p> <p>Exptl. heat of combustion data^[185]:</p> <table border="1"> <tr> <td>$-\Delta U_{B/M}$ (cal/g)</td><td>$-\Delta U_B$ (kcal/mol)</td><td>$-\Delta U_R$ (kcal/mol @ 1 atm. and constant vol.)</td><td>$-\Delta H_R$ (kcal/mol @ 1 atm. and constant pressure)</td></tr> <tr> <td>3,598.67 ± 3.18</td><td>817.38</td><td>816.23</td><td>814.30</td></tr> </table>			$-\Delta U_{B/M}$ (cal/g)	$-\Delta U_B$ (kcal/mol)	$-\Delta U_R$ (kcal/mol @ 1 atm. and constant vol.)	$-\Delta H_R$ (kcal/mol @ 1 atm. and constant pressure)	3,598.67 ± 3.18	817.38	816.23	814.30
$-\Delta U_{B/M}$ (cal/g)	$-\Delta U_B$ (kcal/mol)	$-\Delta U_R$ (kcal/mol @ 1 atm. and constant vol.)	$-\Delta H_R$ (kcal/mol @ 1 atm. and constant pressure)								
3,598.67 ± 3.18	817.38	816.23	814.30								
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.								
$-\Delta_{ex}U^\circ$ [kJ kg ⁻¹]	5,033	<p>4,587 (ZMWCyw)^[20]</p> <p>3,975^[10]</p> <p>1.29 kcal/g (Q_{max} calcd.)^[81]</p> <p>692 cal/g (@ 1.619 g cm⁻³)^[104]</p> <p>3,766 (calcd., ICT-code)^[105]</p> <p>840 kcal/kg (@ 1.000 g cm⁻³, calcd.) [H₂O vapor]^[108]</p> <p>990 kcal/kg (@ 1.600 g cm⁻³, calcd.) [H₂O vapor]^[108]</p> <p>E_0 = 7.0 GPa^[114]</p> <p>1.41 kcal/g (max. calcd. value) [H₂O (l)]^[27]</p>	<p>4,564 [H₂O (l)]^[1, 16]</p> <p>3,646 [H₂O (g)]^[1]</p> <p>1,080 kcal/kg^[23, 28, 33]</p> <p>4,561 (@ 1.53 g cm⁻³) [H₂O (l)], (calorimetric heat of det., Ornellas method, 25 g cylinder sample, 1.2 cm diameter, detonated in isothermal calorimetry bomb under 65 Pa vacuum)^[87]</p> <p>780 cal/g (@ 1.69 g cm⁻³, cast TNT)^[96]</p> <p>4,350 J/g (@ 1.632 g cm⁻³, det. energy, cylinder test)^[100]</p> <p>860 kcal/kg (@ 1.000 g cm⁻³) [H₂O vapor]^[108]</p>								

		<p>1.27 kcal/g (max. calcd. value) [H₂O (g)]^[27]</p> <p>5.26 MJ/kg (calcd., SD method)^[164]</p>	<p>1,030 kcal/kg (@ 1.600 g cm⁻³, calcd.) [H₂O vapor]^[108]</p> <p>4,576 J/g (@ 1.533 g cm⁻³, heat of det., heavily confined charge) [H₂O (l)]^[100]</p> <p>4,382 J/g (@ 1.533 g cm⁻³, heat of det., heavily confined charge) [H₂O (g)]^[100]</p> <p>$E_0 = 6,830 \text{ MJ/m}^3$ (detonation energy est. based on cylinder test, @ 1.59 g cm⁻³)^[113]</p> <p>$E_0^{\text{cal}} = 6.50 \text{ GPa}$ (calcd. from cylinder test data)^[114]</p> <p>1,030 kcal/kg (@ 1.60 g cm⁻³, Q_{exp})^[134]</p> <p>1.09 kcal/g (@ 1.54 g cm⁻³) [H₂O (l)]^[27]</p> <p>1.02 kcal/g (@ 1.54 g cm⁻³) [H₂O (g)]^[27]</p> <p>1,010 kcal/kg^[163]</p> <p>1,080 cal/g (cast TNT)^[165]</p>
T_{ex} [K]	3,462	<p>3,000 (@ 1.0 g cm⁻³)^[27]</p> <p>3,450 (@ 1.59 g cm⁻³)^[27]</p> <p>4,417 (@ 1.5 g cm⁻³)^[28]</p> <p>2,757 (@ 1.650 g cm⁻³, calcd.)^[28]</p> <p>2,736 (@ 1.65 g cm⁻³, calcd.)^[28]</p> <p>3,563 (@ 1.64 g cm⁻³, calcd.)^[74]</p> <p>2,512 (calcd., ICT-code)^[105]</p>	<p>2,820^[10]</p> <p>2,800 °C^[49]</p> <p>3,000 (@ 1.0 g cm⁻³)^[27]</p> <p>3,450 (@ 1.59 g cm⁻³)^[27]</p> <p>3,100 °C^[163]</p>

		<p>3,238 (@ 100% TMD, calcd., Cheetah-6)^[133]</p> <p>2,937 (@ 1.60 g cm⁻³, $\Delta H_f^0 = -26.5$ kJ/kg, calcd., FORTRAN BKW)^[154]</p> <p>3,175 (@ 1.061 g cm⁻³, $\Delta H_f^0 = -26.5$ kJ/kg, calcd., FORTRAN BKW)^[154]</p> <p>3,080 (@ 0.732 g cm⁻³, $\Delta H_f^0 = -26.5$ kJ/kg, calcd., FORTRAN BKW)^[154]</p> <p>3,647 K (calcd., SD method)^[164]</p> <p>3,092 (@ 1.654 g cm⁻³, $\Delta H_f = -63$ kJ/mol, calcd., JAGUAR)^[174]</p>	
p_{C-I} [kbar]	206	<p>192 (@ 1.64 g cm⁻³) (CHEETAH 2.0)^[11]</p> <p>183 (@ 1.61 g cm⁻³) (CHEETAH 2.0)^[11]</p> <p>207 (@ 1.654 g cm⁻³, calcd., K-J)^[50]</p> <p>154 (@ 1.59 g cm⁻³, calcd.)^[28]</p> <p>187.2 (@ 1.622 g cm⁻³, calcd.)^[28]</p> <p>225 (@ 1.640 g cm⁻³, calcd.)^[28]</p> <p>222 (@ 1.65 g cm⁻³, calcd.)^[28]</p> <p>166 (@ 1.63–1.64 g cm⁻³, calcd., R-P method)^[59]</p> <p>45 (@ 0.73 g cm⁻³, calcd., BKW)^[60]</p> <p>19.4 GPa (@ TMD, calcd., CHEETAH 2.0)^[61]</p>	<p>190 (@ 1.64 g cm⁻³)^[11, 27]</p> <p>187 (@ 1.61 g cm⁻³)^[11]</p> <p>202 (@ 1.59 g cm⁻³)^[27]</p> <p>190 (@ 1.63 g cm⁻³)^[27]</p> <p>222 (@ 1.65 g cm⁻³)^[27]</p> <p>18.91 ± 0.1 GPa (@ 1.637 g cm⁻³)^[25]</p> <p>202 (@ 1.59 g cm⁻³, pressed)^[28]</p> <p>190 (@ 1.640 g cm⁻³, pressed)^[28]</p> <p>189 × 10³ atm. (@ 1.64 g cm⁻³)^[28]</p> <p>178 (@ 1.64 g cm⁻³)^[33]</p> <p>182 (@ 1.64 g cm⁻³, @ 93 °C, liq.)^[44]</p> <p>205^[59]</p>

		<p>64 (@ 0.95 g cm⁻³, calcd., K-J)^[63]</p> <p>72 (@ 1.0 g cm⁻³, calcd., K-J)^[63]</p> <p>193 (@ 1.59 g cm⁻³, calcd., K-J)^[63]</p> <p>96 (@ 1.14 g cm⁻³, calcd., K-J)^[63]</p> <p>127 (@ 1.30 g cm⁻³, calcd., K-J)^[63]</p> <p>159 (@ 1.45 g cm⁻³, calcd., K-J)^[63]</p> <p>214 (@ 1.63 g cm⁻³, calcd., K-J)^[63]</p> <p>201 (@ 1.62 g cm⁻³, calcd., K-J)^[63]</p> <p>204 (@ 1.63 g cm⁻³, calcd., K-J)^[63]</p> <p>80 (@ 1.051 g cm⁻³, calcd., K-J)^[63]</p> <p>36.4 (@ 0.8 g cm⁻³, calcd., thermochem.)^[64]</p> <p>62.5 (@ 1.0 g cm⁻³, calcd., thermochem.)^[64]</p> <p>110 (@ 1.061 g cm⁻³, calcd., thermochem.)^[64]</p> <p>122.2 (@ 1.36 g cm⁻³, calcd., thermochem.)^[64]</p> <p>142 (@ 1.45 g cm⁻³, calcd., thermochem.)^[64]</p> <p>176.5 (@ 1.59 g cm⁻³, calcd., thermochem.)^[64]</p>	<p>62.2 (@ 0.95 g cm⁻³)^[63]</p> <p>76.3 (@ 1.0 g cm⁻³)^[63]</p> <p>179.0 (@ 1.59 g cm⁻³)^[63]</p> <p>94 (@ 1.14 g cm⁻³)^[63]</p> <p>123 (@ 1.30 g cm⁻³)^[63]</p> <p>162 (@ 1.45 g cm⁻³)^[63]</p> <p>177 (@ 1.63 g cm⁻³)^[63]</p> <p>210 (@ 1.62 g cm⁻³)^[63]</p> <p>225 (@ 1.63 g cm⁻³)^[63]</p> <p>115 (@ 1.051 g cm⁻³)^[63]</p> <p>40.5 (@ 0.8 g cm⁻³)^[64]</p> <p>63.4 (@ 1.0 g cm⁻³)^[64]</p> <p>71.8 (@ 1.061 g cm⁻³)^[64]</p> <p>124.7 (@ 1.36 g cm⁻³)^[64]</p> <p>144.6 (@ 1.45 g cm⁻³)^[64]</p> <p>182.4 (@ 1.59 g cm⁻³)^[64]</p> <p>197.1 (@ 1.64 g cm⁻³)^[64]</p> <p>192 (@ 1.69 g cm⁻³, cast TNT)^[96]</p> <p>1,840 kg/cm² (@ 0.20 g cm⁻³ loading ρ, measured by piston and obturator)^[93]</p> <p>2,625 kg/cm² (@ 0.25 g cm⁻³ loading ρ, measured by piston and obturator)^[93]</p>
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		<p>190 (@ 1.64 g cm⁻³, calcd., thermochem.)^[64]</p> <p>19.6 GPa (@ 1.64 g cm⁻³, CHEETAH, 1998)^[54]</p> <p>20.75 GPa (@ 1.654 g cm⁻³, calcd., CHEETAH 3)^[73]</p> <p>163.4 (@ 1.64 g cm⁻³, calcd.)^[74]</p> <p>207 (@ 1.654 g cm⁻³, calcd.)^[81]</p> <p>187 (@ 1.619 g cm⁻³)^[104]</p> <p>103.3 MPa (calcd., ICT-code)^[105]</p> <p>19.6 GPa (@ 1.640 g cm⁻³, $\Delta H_f^\circ = -59.4$ kJ/mol, calcd., Cheetah)^[131]</p> <p>198 (@ 100% TMD, calcd., Cheetah-6)^[133]</p> <p>20.6 GPa (@ 1.60 g cm⁻³, $\Delta H_f^\circ = -26.5$ kJ/kg, calcd., FORTRAN BKW)^[154]</p> <p>8.5 GPa (@ 1.061 g cm⁻³, $\Delta H_f^\circ = -26.5$ kJ/kg, calcd., FORTRAN BKW)^[154]</p> <p>4.5 GPa (@ 0.732 g cm⁻³, $\Delta H_f^\circ = -26.5$ kJ/kg, calcd., FORTRAN BKW)^[154]</p> <p>0.2066 Mbar (@ 1.64 g cm⁻³, calcd. empirical eqn.)^[165]</p> <p>0.190 Mbar (@ 1.58 g cm⁻³, calcd. empirical eqn.)^[165]</p>	<p>3,675 kg/cm² (@ 0.30 g cm⁻³ loading ρ, measured by piston and obturator)^[93]</p> <p>20.5 GPa (@ 1.632 g cm⁻³)^[100]</p> <p>21.0 GPa (@ 1,630 kg/m³, cylinder test)^[114]</p> <p>19.0 GPa (@ 1.60 g cm⁻³)^[154]</p> <p>11.0 GPa (@ 1.061 g cm⁻³)^[154]</p> <p>5.9 GPa (@ 0.732 g cm⁻³)^[154]</p> <p>20.5 GPa (@ 1.632 g cm⁻³)^[155]</p> <p>0.177 Mbar (@ 1.64 g cm⁻³)^[165]</p> <p>0.177 Mbar (@ 1.58 g cm⁻³)^[165]</p> <p>0.170 Mbar^[165]</p>
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		<p>0.026 Mbar (@ 0.0624 g cm⁻³, calcd. empirical, eqn.)^[165]</p> <p>19.8 GPa (@ 1.654 g cm⁻³, $\Delta H_f = -63$ kJ/mol, calcd., JAGUAR)^[174]</p>	
VoD [m s ⁻¹]	7,224	<p>6,700 (@ 1.57 g cm⁻³)^[10]</p> <p>6,843 (@ 1.64 g cm⁻³) (CHEETAH 2.0)^[11]</p> <p>6,752 (@ 1.61 g cm⁻³) (CHEETAH 2.0)^[11]</p> <p>6,970 (@ 1.60 g cm⁻³, average value from lit.)^[43]</p> <p>7,020 (@ 1.654 g cm⁻³, calcd., K-J)^[50]</p> <p>7,290 (@ 1.65 g cm⁻³, calcd.)^[28]</p> <p>6,825 (@ 1.56 g cm⁻³, calcd.)^[33]</p> <p>6,670 (@ 1.65 g cm⁻³ (TMD), calcd., R-P method)^[59]</p> <p>7,230 (@ 1.65 g cm⁻³ (TMD), calcd., <i>Aizenshtadt</i>)^[59]</p> <p>6,990 (@ 1.65 g cm⁻³ (TMD), calcd., K-J)^[59]</p> <p>4,500 (@ 0.73 g cm⁻³, calcd., BKW)^[60]</p> <p>6,900 (@ TMD, calcd., CHEETAH 2.0)^[61]</p> <p>7,192 (@ TMD, calcd., CHEETAH v8.0)^[62]</p>	<p>6,950 (@ 1.64 g cm⁻³)^[11, 15]</p> <p>6,780 (@ 1.61 g cm⁻³)^[11]</p> <p>6,930 (@ 1.64 g cm⁻³)^[14]</p> <p>6,500 (@ 1.45 g cm⁻³)^[14]</p> <p>6,200 (@ 1.36 g cm⁻³)^[14]</p> <p>5,000 (@ 1.0 g cm⁻³)^[14]</p> <p>4,340 (@ 0.8 g cm⁻³)^[14]</p> <p>6,640 (@ 1.56 g cm⁻³, cast)^[17]</p> <p>6,824 (@ 1.72 g cm⁻³, pressed)^[17]</p> <p>6,860 (@ 1.63 g cm⁻³)^[19, 65]</p> <p>6,825 (@ 1.56 g cm⁻³, 1.0 in charge diameter, pressed, unconfined)^[23]</p> <p>6,640 (@ 1.56 g cm⁻³, 1.0 in charge diameter, cast, unconfined)^[23]</p> <p>6,633 (@ 1.462 g cm⁻³, @ 81 °C, liquid TNT)^[25]</p> <p>6,942 ± 16 (@ 1.637 g cm⁻³)^[25]</p> <p>6,940 (@ 1.59 g cm⁻³, pressed)^[28]</p>

		4,340 (@ 0.8 g cm ⁻³ , calcd., thermochem.) ^[64]	6,950 (@ 1.640 g cm ⁻³ , pressed) ^[28]
		5,100 (@ 1.0 g cm ⁻³ , calcd., thermochem.) ^[64]	6,790 (@ 1.622 g cm ⁻³ , pressed) ^[28]
		5,254 (@ 1.061 g cm ⁻³ , calcd., thermochem.) ^[64]	7,361 (@ 1.640 g cm ⁻³ , pressed) ^[28]
		6,200 (@ 1.36 g cm ⁻³ , calcd., thermochem.) ^[64]	6,970 (@ 1.59 g cm ⁻³ (cast)) ^[43]
		6,500 (@ 1.45 g cm ⁻³ , calcd., thermochem.) ^[64]	6,700 (@ 1.60 g cm ⁻³) ^[49]
		6,940 (@ 1.59 g cm ⁻³ , calcd., thermochem.) ^[64]	7,128 (calcd. based on sand experiment) ^[43]
		6,950 (@ 1.64 g cm ⁻³ , calcd., thermochem.) ^[64]	6,950 (@ 1.64 g cm ⁻³ , @ 93 °C, liq.) ^[44]
		6,886 (@ 1.64 g cm ⁻³ , CHEETAH 1998) ^[54]	6,990 (est. LASEM method) ^[62]
		7,236 (@ 1.654 g cm ⁻³ , calcd., CHEETAH 3) ^[73]	7,026 (@ TMD, measured using large-scale detonation test) ^[62]
		7,060 (@ 1.64 g cm ⁻³ , calcd.) ^[74]	3,910 (@ 0.76 g cm ⁻³ , aquarium test data, clay pipe, 10 cm, TNT flakes) ^[60]
		7,010 (@ 1.654 g cm ⁻³ , calcd.) ^[81]	4,290 (@ 0.85 g cm ⁻³ , aquarium test data, clay pipe, 10 cm, TNT flakes) ^[60]
		6,700 (@ 1.619 g cm ⁻³) ^[104]	
		5,110 (@ 1 g cm ⁻³ , calcd., Kamlet method) ^[110]	4,542 (@ 0.8 g cm ⁻³) ^[64]
		6,840 (@ 1.6 g cm ⁻³ , calcd., Kamlet method) ^[110]	512 (@ 1.0 g cm ⁻³) ^[64]
		4,910 (@ 1 g cm ⁻³ , calcd., Urizar method) ^[110]	5,282 (@ 1.061 g cm ⁻³) ^[64]
		6,960 (@ 1.6 g cm ⁻³ , calcd., Urizar method) ^[110]	6,124 (@ 1.36 g cm ⁻³) ^[64]
			6,382 (@ 1.45 g cm ⁻³) ^[64]
			6,774 (@ 1.59 g cm ⁻³) ^[64]

		<p>6,886 (@ 1.640 g cm⁻³, $\Delta H_f^0 = -59.4$ kJ/mol, calcd., Cheetah)^[131]</p> <p>6,480 (@ 1.50 g cm⁻³, K-W eqn.)^[146]</p> <p>6,950 (@ 1.60 g cm⁻³, $\Delta H_f^0 = -26.5$ kJ/kg, calcd., FORTRAN BKW)^[154]</p> <p>5,339 (@ 1.061 g cm⁻³, $\Delta H_f^0 = -26.5$ kJ/kg, calcd., FORTRAN BKW)^[154]</p> <p>4,511 (@ 0.732 g cm⁻³, $\Delta H_f^0 = -26.5$ kJ/kg, calcd., FORTRAN BKW)^[154]</p> <p>0.695 cm/μs (@ 1.64 g cm⁻³, calcd., empirical eqn.)^[165]</p> <p>6,890 (@ 1.654 g cm⁻³, $\Delta H_f = -63$ kJ/mol, calcd., JAGUAR)^[174]</p>	<p>6,918 (@ 1.64 g cm⁻³)^[64]</p> <p>6,940 (@ 1.64 g cm⁻³)^[74]</p> <p>7,000 (@ 1.615 g cm⁻³, Dautriche method, loaded in Cu tubes, 10 mm diameter, compressed under pressure of 2,500 kg/cm²)^[89]</p> <p>6,780 (@ 1.69 g cm⁻³, cast TNT)^[96]</p> <p>4,450 (@ 0.90 g cm⁻³, half-meter lengths, extra light Pb tubing, 5 in internal diameter, 12 ounces per foot)^[89]</p> <p>7,028 (cast TNT)^[93]</p> <p>4,961 (compressed, @ 0.909 g cm⁻³)^[93]</p> <p>7,140 (max. VoD, @ 1.60 g cm⁻³, 10 pellets, paper cartridge, exploded by primer of 0.5 g fulminate and 25 g Dynamite)^[93]</p> <p>6,913 (@ 1.60 g cm⁻³)^[98]</p> <p>7,070 (@ 1.632 g cm⁻³)^[100]</p> <p>5,940 (@ 1.34 g cm⁻³, charges of 21 mm diameter, initiated by 2 g detonator in the open)^[88]</p> <p>6,400 (@ 1.45 g cm⁻³, charges of 21 mm diameter, initiated by 2 g detonator in the open)^[88]</p> <p>6,590 (@ 1.50 g cm⁻³, charges of 21 mm diameter, initiated by 2 g detonator in the open)^[88]</p>
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			<p>6,680 (@ 1.60 g cm⁻³, charges of 21 mm diameter, initiated by 2 g detonator in the open)^[88]</p> <p>2,385 (@ 0.25 g cm⁻³, metal pipe, 10–15 mm diameter)^[88]</p> <p>3,100 (@ 0.56 g cm⁻³, metal pipe, 10–15 mm diameter)^[88]</p> <p>4,100 (@ 0.83 g cm⁻³, metal pipe, 10–15 mm diameter)^[88]</p> <p>4,720 (@ 1.21 g cm⁻³, metal pipe, 10–15 mm diameter)^[88]</p> <p>6,990 (@ 1.62 g cm⁻³, metal pipe, 10–15 mm diameter)^[88]</p> <p>4,720 (@ 1.21 g cm⁻³, charges in bakelite pipe of 4.5–8.2 mm internal diameter)^[88]</p> <p>5,900 (@ 1.40 g cm⁻³, charges in bakelite pipe of 4.5–8.2 mm internal diameter)^[88]</p> <p>7,400 (@ 1.52 g cm⁻³, charges in bakelite pipe of 4.5–8.2 mm internal diameter)^[88]</p> <p>5,250 (@ 1.10 g cm⁻³, charges in steel pipe, 31.7 mm diameter)^[88]</p> <p>6,930 (@ 1.62 g cm⁻³, charges in steel pipe, 31.7 mm diameter)^[88]</p>
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			<p>5,060 (@ 1 g cm⁻³)^[110]</p> <p>6,970 (@ 1.6 g cm⁻³)^[110]</p> <p>6,910 (@ 1.59 g cm⁻³)^[113]</p> <p>6,930 (@ 1,630 kg/m³, cylinder test)^[114]</p> <p>7,090 (@ 1.65 g cm⁻³)^[120]</p> <p>6,910 (@ 1.590 g cm⁻³, cylinder test, impulse X-ray apparatus, 300 mm long tube, 25 mm internal diameter, 2.5 mm wall thickness)^[129]</p> <p>6,900 (@ 1.6 g cm⁻³)^[130]</p> <p>22,500 ft/s (@ 1.6 g/mL)^[142]</p> <p>6,700 (@ 1.50 g cm⁻³)^[146]</p> <p>6,900 (@ 1.56 g cm⁻³)^[149]</p> <p>6,950 (@ 1.60 g cm⁻³)^[154]</p> <p>5,254 (@ 1.061 g cm⁻³)^[154]</p> <p>4,200 (@ 0.732 g cm⁻³)^[154]</p> <p>7,070 (@ 1.632 g cm⁻³)^[155]</p> <p>7,000 (@ 1.62 g cm⁻³)^[163]</p> <p>6,574 (@ 1.46 g cm⁻³, D_i) (D_i = ideal detonation velocity)^[164]</p> <p>6,510 (@ 1.46 g cm⁻³, D_f) (D_f = detonation velocity for critical detonation diameter)^[164]</p> <p>0.695 cm/μs (@ 1.64 g cm⁻³)^[165]</p>
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			0.688 cm/ μ s (@ 1.58 g cm ⁻³) ^[165] 0.380 cm/ μ s (@ 0.624 g cm ⁻³) ^[165] 6,950 (@ 1.57 g cm ⁻³) ^[171]
V_0 [L kg ⁻¹]	634	717 (ZMWCyw) ^[20] 690 (@ 0 °C) ^[10]	730 ^[23, 163] 825 ^[1, 24] 684 (@ 1.62 g cm ⁻³) ^[27] 690 (@ 1.64 g cm ⁻³) ^[27] 610 [H ₂ O (l)] (ρ = 1.5 g cm ⁻³ , Dolgov bomb) ^[31, 32] 750 [H ₂ O (g)] (ρ = 1.5 g cm ⁻³ , Dolgov bomb) ^[31, 32] 690 (@ 0 °C, 760 mm Hg) ^[49] 730 (cast TNT) ^[165]

Plate push value @ 98% TMD = 2,930 ft/s (cast TNT)^[96], plate push value @ 93% TMD = 2,830 ft/s (measured with cast TNT powder pressed to 93% TMD)^[96], failure diameter = 2.69 cm (cast TNT)^[96], failure diameter of pressed TNT @ 98% TMD is ¹/10th this value^[96]

Effect of temperature on rate of detonation^[23]:

T of charge (°C)	-54	21	60	60
Hours at T	16	16	24	72
Density, g/cc	1.63	1.62	1.64	1.64
Rate (m/s)	6,700	6,820	6,770	6,510

Calculated using hydrodynamic theory of detonation equations (*Caldirola*)^[28]:

ρ of charge (g cm ⁻³)	Detonation pressure (kg/cm ²)	Detonation temp. (K)
1.00	68,700	3,210
1.29	132,800	3,610
1.46	178,000	3,860
1.59	216,200	4,020

Exptl. values (*Mason and Gibson*)^[28]:

$\rho = 0.70$ g cm⁻³, temp. of detonation = no detonation^[28]

$\rho = 1.5$ g cm⁻³, temp. of detonation = 4,417 K^[28]

Exptl. values (radiation method)^[28]:

$\rho = 0.70$ g cm⁻³, temp. of detonation = 3,650 K^[28]

$\rho = 1.15$ g cm⁻³, temp. of detonation = 4,350 K^[28]

$\rho = 1.5$ g cm⁻³, temp. of detonation = 4,750 K^[28]

Calcd. (based on hydrodynamic theory)^[28]:

Loading $\rho = 1.50$ g cm⁻³, temp. of detonation = 3,600 °C, pressure (10 atm.) = 1.10, VoD = 6,480 m/s^[28]

T of detonation by radiation method for TNT powders (exptl. values)^[28]:

Average particle diameter (microns)	ρ / g cm ⁻³	Average T (K)
5	0.75	4,610
5	1.55	4,960
800 (20 mesh)	1.54	5,320

Luminosity method (exptl.), radiation slit width = 1 m, unsheathed explosions in air^[28]:

TNT loading $\rho = 1.29$ g cm⁻³, Average $T_{\text{det.}}$ = 4,850 K^[28]

TNT loading $\rho = 1.56$ g cm⁻³, Average $T_{\text{det.}}$ = 5,500 K^[28]

Radiation T observed without slit aperture, for interval after detonation of 18 ms: loading $\rho = 1.56$ g cm⁻³, average $T = 4,840$ K^[28]

Exptl. VoD values using sweep trace of cathode ray tube by electrical signals (separation of signal stations = 10 cm, station 1 located 5 cm from detonator, charge diameter = 1.92 cm)^[28]:

Average particle diameter (microns)	ρ (g cm ⁻³)	VoD (m/s)
5	0.75	3,660
5	1.55	6,630
800 (20 mesh)	0.97	Incomplete detonation
800	1.54	6,700

Exptl. VoD values after storing TNT (charges = sticks of 1-¹/₈ in in diameter, 18 in long, drum camera apparatus)^[28]:

Cast TNT, 16 h storage @ -65°F, $\rho = 1.63$ g cm⁻³, det. rate = 6,700 m/s^[28]

Cast TNT, 16 h storage @ +70°F, $\rho = 1.62$ g cm⁻³, det. rate = 6,820 m/s^[28]

Cast TNT, 24 h storage @ +140°F, $\rho = 1.64$ g cm⁻³, det. rate = 6,770 m/s^[28]

Cast TNT, 72 h storage @ +140°F, $\rho = 1.64$ g cm⁻³, det. rate = 6,510 m/s^[28]

Exptl. determined VoD of compressed charges of TNT (@ different ρ and different diameter sizes (no units given))^[28]:

ρ (g/cc)	VoD (m/s)		
	0.75	1.0	1.75
1.53	6,830	6,920	7,000
1.40	6,350	6,450	6,510
1.34	6,150	6,180	6,210

Exptl. determined VoD for TNT in different confining vessels^[28]:

Charge ρ (g/cc)	Vessel type	Diameter of charge (mm)	Wall thickness (mm)	VoD (m/s)
0.250 (TNT powder)	Glass	25	1	2,363
0.250 (TNT powder)	Steel	27	4	2,478
0.832 (TNT powder)	Glass	16	0.8	3,308
0.832 (TNT powder)	Copper	15	1	4,100

1.6 (TNT cast)	Steel	21	3	6,650
1.6 (TNT cast)	Steel	29	10	6,700
1.6 (TNT cast)	Steel	160	25	6,690
1.6 (TNT cast)	Steel	300	50	6,710

Exptl. determined VoD at different temperatures ($\rho = 0.90 \text{ g cm}^{-3}$, powdery samples in thin-walled Pb tubes with 12.5 mm diameter)^[28]:

VoD @ 25 °C (m/s)	VoD @ -80 °C (m/s)	VoD @ -180 °C (m/s)
4,310	4,800	4,550
4,460	4,230	4,570
4,580	4,250	4,800
Av. value = 4,450	Av. value = 4,430	Av. value = 4,640

Exptl. determined values^[32]: detonation pressure = 220 kbar, bulk specific gravity = 1.64, VoD = 6,930 m/s, heat of detonation = 1,102 cal/g^[32]

Exptl. determined gas pressures (by exploding samples in small bombs, pressure measured by piston and obturator)^[32]:

Loading $\rho = 0.20 \text{ g cm}^{-3}$, $P = 1,840 \text{ kg/cm}^2$ ^[32]

Loading $\rho = 0.25 \text{ g cm}^{-3}$, $P = 2,625 \text{ kg/cm}^2$ ^[32]

Loading $\rho = 0.30 \text{ g cm}^{-3}$, $P = 3,675 \text{ kg/cm}^2$ ^[32]

VoD = 6.91 m/s (@ $1.60 \pm 0.01 \text{ g cm}^{-3}$, granular TNT, 90% passes through a no. 50 screen, average particle size = 200 μ , batch pressed isostatically @ 30,000 psi); VoD value is within 0.02 mm/ μ s of all generally accepted infinite diameter values^[68]

Detonation parameters of cast and pressed TNT (exptl. determined using oscilloscope)^[68]:

	Pressed TNT	Cast TNT
ρ (g/cc)	1.60 ± 0.01	1.62 ± 0.01
VoD (mm/ μ s)	6.91	6.85
C-J particle velocity (mm/ μ s)	1.72	1.60
p_{CJ} (kbar)	190	178
Reaction time, r_{CJ} (ns)	141	300

Comparison of detonation parameters for pressed TNT^[68]:

Parameter	Results from ^[68]	Dremin values ^[68]	Craig values ^{[68]†}	
			First break	Second break
ρ (g/cc)	1.60	1.59	1.63	1.63
VoD (mm/ μ s)	(6.91)	6.91	(6.94) [‡]	(6.94) [‡]
U_{CJ} (mm/ μ s)	1.72 ± 0.05	1.62 ± 0.08	(1.84)	(1.63)
P_{CJ} (kbar)	190	178	208.5	184.5
r_{CJ} (ns)	141 ± 30	<100		

[†] = results for 50.8 mm diameter; [‡] = calculated from equations

For essentially voidless materials of $\geq 95\%$ TMD, the VoD @ critical conditions (D_c) is less than the ideal detonation velocity (D_i), but it is only slightly less @ high % TMD^[70], however, high porosity, granular charges show much lower D_c/D_i values^[70]:

Pressed-TNT @ 98% TMD, $D_c/D_i = 0.95$ ^[70]

Cast-TNT @ 98% TMD, $D_c/D_i = 0.94$ ^[70]

Granular TNT @ 50% TMD, $D_c/D_i = 0.65$ ^[70]

Calorimetric heat of det., Ornellas method, 25 g cylinder sample, 1.2 cm diameter, detonated in iso-thermal calorimetry bomb under 65 Pa vacuum^[87]:

ρ (g cm ⁻³)	J/g (25 °C, H ₂ O (l))	J/cm ³	J/cm ³ (TMD)
1.53	4,561	6,987	7,544

Chapman–Jouguet pressure, energy and isentropic exponent from H₂O-shock measurements^[104]:

ρ (g cm ⁻³)	D (m/s)	$U_{\text{H}_2\text{O}}$ (m/s)	$u_{\text{H}_2\text{O}}$ (m/s)	$P_{\text{H}_2\text{O}}$ @ HE•H ₂ O interface (kb)	$p_{\text{C-J}}$ (kb)	k	Q (cal/g)
1.62	6,790	5,532	2,312	127.6	187.2	2.99	692

Variation of VoD with cartridge diameter, TNT powder^[146]:

Diameter (cm)	VoD (m/s)	Diameter (cm)	VoD (m/s)
1.9	3,190	10.2	4,560
3.2	3,680	12.7	–
5.1	4,060	15.2	4,815
6.4	4,030	21.6	–
7.6	4,100		

Exptl. VoD of pressed TNT charges (with ρ close to that of the single crystal), * in the series of expts. with $\rho_0 = 1.63 - 1.645$ g cm⁻³, quenching of the detonation was observed, quenching of detonation also observed when detonation initiated by intermediate pressed TNT detonators with $d = 8$ mm, $h = 15$ mm and $\rho_0 = 1.6$ g cm⁻³; † indicates failure to detonate^[148]:

d (mm)	ρ_0 (g cm ⁻³)	D (m/s)	n	σ_i (m/s)	d (mm)	ρ_0 (g cm ⁻³)	D (m/s)	n	σ_i (m/s)
13	1.59	6,850	5	+100 –40	8	1.62– 1.63	6,670	3	+40 –60
13	1.6	6,870	4	+30 –40	8*	1.63– 1.64	6,480	3	+70 –50
13	1.61	6,870	4	+20 –90	8*	1.639– 1.641	6,350	1	
13	1.62	6,900	4	+25 –35	8*	1.644– 1.645	6,450		
13	1.64	6,950	3	+30 –50	8†	1.645– 1.65			
13	1.65	6,800	3	+50 –40	8†	1.642– 1.644		1	
10	1.61	6,790	3	+60 –90	8†	1.640– 1.65		1	
10	1.62	6,830	3	+25 –61	8†	1.64– 1.645		2	

10	1.64	6,790	3	+50 -100	8 [†]	1.64- 1.645		1	
10	1.642- 1.646	6,725	1	-	8 [†]	1.65- 1.659		1	
10	1.647- 1.65	6,730	1	-	6	1.63- 1.64			
8	1.61-1.62	6,650	3	+30 -					

Exptl. VoD of pressed TNT charges (with ρ close to that of the single crystal) as a function of the diameter of the pressed TNT charges^[148]:

ρ_0 (g cm ⁻³)	d (mm)	D (m/s)
1.625	8	6,670
	10	6,830
	13	6,910
	8	6,580
1.630	10	6,830
	13	6,930
	8	6,480
1.635	10	6,820
	13	6,945

VoD of cylindrical charges, cellophane tube of 3.17 cm diameter, 30 cm long, unconfined, TNT powder (98.5% purity), 98% passed through no. 25 BSS sieve and remained on no. 120, cartridges primed with 7 g Tetryl pellet and No. 6 copper detonator, $\rho = 1.00$ g cm⁻³, no. of shots fired = 12, measured VoD values (m/s)^[150]: 4,675, 4,660, 4,656, 4,651, 4,646, 4,644, 4,644, 4,643, 4,642, 4,639, 4,638, 4,632, mean value = 4,650 m/s^[150]

VoD of cast TNT: (i) poured clear, (ii) poured cloudy and (iii) creamed. Charges of 3.17 cm diameter, 40 cm long, unconfined. Poured-cloudy cast TNT always detonated under conditions used, creamed castings always detonated under conditions used but poured-clear castings could only be detonated without confinement only in some cases. A 7 g Tetryl primer was used for creamed castings and a 28 g Tetryl primer for poured-cloudy^[150]:

TNT	Batch A		Batch C	
	Set point = 80.32 °C		Set point = 80.45 °C	
Casting method	Poured-clear	Creamed	Poured-cloudy	Creamed
ρ (g cm ⁻³)	1.605	1.625	1.620	1.625
Mean VoD (m/s)	6,430	6,850	6,880	6,880
No. of determinations	5	6	6	12
Range	630	61	50	50
Standard deviation	–	23	18	15
Standard error	–	9	7	4

VoD for various batches of TNT, creamed castings, 3.17 cm diameter, 40 cm long, $\rho = 1.625$ g cm⁻³^[150]:

Batch	A	B	C	D	E	F
Set point (°C)	80.32	80.40	80.45	80.50	80.66	80.86
Purity (approx. %)	98.8	99.0	99.1	99.2	99.5	99.8
Mean VoD (m/s)	6,850	6,850	6,880	6,900	6,940	6,950
No. determinations	14	10	24	18	6	6
Range	61	94	62	35	42	59
Standard deviation	18	27	17	12	16	22
Standard error	5	9	4	3	7	9

Different diameters of cast TNT: poured-clear, poured-cloudy and creamed, set point 80.50 °C; unconfined, length = 50 cm, * = 40 cm long^[150]:

Charge diameter (cm)	1.26	1.66	1.90	2.20	2.54	3.17*
TNT poured-clear						No detonation
TNT poured-cloudy; Density (g/cm ³)						
Measured velocities (m/s)					1.615	1.620
				No detonation	6,698	6,919
					6,681	6,915
					6,681	6,910
					6,637	6,905
					6,562	6,898
					6,560	6,890
					6,640	6,910
Mean velocity					6,640	6,910
Range					138	29
Standard deviation					62	11
Standard error					25	4
TNT creamed Density (g/cm ³)						
Measured velocities (m/s)	No detonation	1.605	1.610	1.615	1.615	1.620
		6,522	6,754	6,854	6,904	6,919
		6,507	6,748	6,846	6,891	6,911
		6,482	6,742	6,814	6,884	6,909
		6,455	6,741	6,812	6,883	6,894
		6,454	6,738	6,810	6,876	6,888
		6,406	6,719	6,801	6,874	6,884
		6,470	6,740	6,820	6,890	6,900
Mean velocity						
Range		116	35	53	30	35
Standard deviation		42	12	22	11	14
Standard error		17	5	9	4	6

Bare and confined charges of creamed TNT, set point 80.45 °C, 3.17 cm in diameter, 40 cm long, density = 1.625 g cm⁻³[150].

	Bare		Confined in steel tube, 0.32 cm wall thickness	
No. of shots fired	12		12	
Measured velocities (m/s)	6,918	6,875	6,916	6,887
	6,897	6,870	6,902	6,883
	6,893	6,869	6,902	6,879
	6,885	6,869	6,901	6,861
	6,884	6,869	6,900	6,860
	6,877	6,868	6,895	6,856
Mean velocity	6,880		6,890	
Range	50 (0.73)		60 (0.87)	
Standard deviation	15 (0.22)		19 (0.27)	
Standard error	4 (0.06)		5 (0.08)	

Effect of confinement in steel tubes of various diameters: poured-clear and creamed TNT, set point 80.50 °C, length = 50 cm; * = tubes preheated to 75 °C for poured-clear and to 50 °C for creamed TNT; † = 40 cm long^[150].

Steel tube internal diameter (cm)	0.94*	0.99	1.29	1.65		2.26	3.17†
Steel tube wall thickness (cm)	0.23	0.18	0.20	0.23	0.08	0.20	0.32
TNT poured clear:							
Density, g/cc	1.590	1.610	1.605	1.605		1.590	1.600
Measured velocities, m/s	6,383	6,794	6,783	6,855		6,867	6,839
	6,343	6,794	6,774	6,835		6,846	6,838
	6,335	6,786	6,769	6,826		6,837	6,825
	6,288	6,781	6,764	6,821		6,817	6,823
	6,225	6,774	6,745	6,817		6,815	6,816
	6,208	6,771	6,742	6,800		6,791	6,809
		6,770	6,736				
		6,768	6,727				
		6,765	6,721				
		6,725	6,700				

Mean velocity	6,300	6,770	6,750	6,830		6,830	6,830
Range	175	60	83	55		76	30
Standard deviation	69	20	26	18		27	12
Standard error	28	6	8	7		11	5
TNT creamed:							
Density, g/cm ³	1.600		1.605	1.605	1.605	1.610	
Measured velocities, m/s	6,659		6,788	6,871	6,804	6,915	
	6,641		6,775	6,866	6,790	6,913	
	6,634		6,773	6,856	6,787	6,913	
	6,630		6,772	6,847	6,782	6,902	
	6,620		6,760	6,822	6,779	6,890	
	6,591		6,735	6,820	6,755	6,887	
	6,630		6,770	6,850	6,780	6,900	
Range	68		53	51	49	28	
Standard deviation	23		18	22	16	12	
Standard error	9		7	9	7	6	

Limit data of diameters and velocities of detonation of cast TNT, set point 80.50 °C^[150]:

Casting		Poured-clear		Poured-cloudy		Creamed	
		Bare	Confined	Bare	Confined	Bare	Confined
Boundary	Diameter (cm)	–	>0.9	2.5	–	1.7	>0.9
	Velocity (m/s)	–	6,300	6,400	–	6,470	6,600
Limiting	Diameter (cm)	–	1.7	~3.0	–	2.7	2.2
	Velocity (m/s)	–	6,830	6,900	6,900	6,900	6,900

Summary of experimental copper cylinder wall velocity data, PETN with a density of 1.763 g/cm³ is the reference explosive, data from^[153]:

Initial density (g/cm ³)	Inner diameter (mm)	Wall thickness (mm)	Wall velocity (mm/μs) at 25.4 mm diameter for R-R ₀ equal to			Velocity-squared cf. with PETN for the same configuration, % comparison R-R ₀ equal to		
			6 mm	12.5 mm	19 mm	6 mm	12.5 mm	19 mm
1.632	50.85	5.186	1.210	1.355	1.410	–39.8	–36.8	–38.0

Summary of code calculations with measure detonation velocities and detonation energies derived from JWL's^[153]:

Initial density (g/cm ³)	PETN-adjusted BKWR Tiger, LLNL library, $\theta = 1,850$ K, at v			JCZ3, LLNL library, v			CHEQ V2.4, at v		
	2.2 mm	4.1 mm	6.5 mm	2.2 mm	4.1 mm	6.5 mm	2.2 mm	4.1 mm	6.5 mm
1.632	3	-1	-1	5	-1	-3	0	-3	-3

Derivation of the total energy of detonation, E_0 from the measured heat of detonation. The final state is assumed to at one atmosphere for all gaseous products including water at 298 K. Code calculated energies with the 1,800 K freeze are also included, data from^[153]:

Measured density (g/cm ³)	Measured confined heat of detonation (kJ/cm ³)	Density from ^[87]	Heat of detonation using density from ^[87]	Energy of detonation, E_0 (kJ/cm ³)			
				From heat of detonation	Freeze at 1,800 K		
					Tiger BKWR	Tiger JCZ3	CHEQ
1.533	-7.01	1.632	-7.46	-7.1	-7.8	-6.1	-7.2

JWL cylinder coefficients data from^[153]:

Initial density, ρ_0 (g/cm ³)	Detonation velocity, D (mm/ μ s)	Energy of detonation, E_0 (kJ/cm ³)	CJ pressure (GPa)	A (GPa)	B (GPa)	C (GPa)	R_1	R_2	ω	γ_{CJ}
1.632	7.07	-7.10	20.5	524.4089	4.900052	0.626131	4.579	0.85	0.23	2.979

Comparison of measured "CJ" temperatures using optical pyrometry^[153]:

Experimental density (g/cm ³)	Max. measured T (K)	Calculated CJ T (K)			Wavelength (μ m)
		Tiger BKWR	Tiger JCZ3	CHEQ	
1.51	3,800–4,000	2,800	3,100	3,800	0.85–0.95
1.2	3,700	2,900	3,200	3,900	0.85–0.95

Critical diameter [cm]	<p>Critical charge diameter influenced by initial ρ, grain size, initial T, crystallinity^[27]</p> <p>Critical heights and diameters^[70]: pressed TNT: $\rho_0 = 1.63 \text{ g cm}^{-3}$; wedge height, $h_c = 2.16 \text{ mm}$ (value for TNT pressed @ 65°C), $d_c = 2.62 \text{ mm}$, d_c (lit. value) = 14, $d_c/h_c = 1.2$^[70], pressed TNT @ $1.62\text{--}1.654 \text{ g cm}^{-3}$ $d_c = 2.62 \pm 0.56 \text{ mm}$^[70], cast TNT @ 1.625 g cm^{-3} (98.2% TMD) $d_c = 22.0\text{--}25.4$^[70], cast TNT @ 1.625 g cm^{-3} (98.2% TMD) $d_c = 26.9 \pm 0.1 \text{ mm}$^[70], $d_c = 2.62 \pm 0.56 \text{ mm}$ (@ 1.62 g cm^{-3}, 97.9% TMD)^[70]</p> <p>$d_c = \sim 3.25 \text{ mm}$ (pressed TNT, $140 \mu\text{m}$ particle size, $\rho = 1.62 \text{ g cm}^{-3}$ (98.0% TMD))^[90], $d_c = \sim 2.5 \text{ mm}$ (pressed TNT, $30 \mu\text{m}$ particle size, $\rho = 1.60 \text{ g cm}^{-3}$ (97.0% TMD))^[90]</p> <p>Effect of different casting techniques on d_c (creamed = melt stirred until it becomes milky due to the formation of small crystals; at this point it is poured into the mold)^[70]:</p> <table><tr><td>Casting method</td><td>d_c (cm)</td></tr><tr><td>Poured, clear</td><td>$3.17 < d_c$</td></tr><tr><td>Creamed</td><td>$2.20 < d_c < 2.54$</td></tr><tr><td>Creamed plus 10% fines</td><td>$1.26 < d_c < 1.66$</td></tr></table> <p>Effect of temperature (critical T) on d_c (granular TNT, $\rho = 1.0 \text{ g cm}^{-3}$, + = steady detonation, – = detonation failure)^[70]:</p> <table><tr><td>T ($^\circ\text{C}$)</td><td>d_c (cm)</td></tr><tr><td>–193</td><td>10 +, ~ 10.5 +, ~ 9.1 –, ~ 9.4 –, ~ 9.7 –</td></tr><tr><td>~ 30</td><td>~ 6.5 +, ~ 6.1 +, ~ 6.0 –</td></tr><tr><td>75</td><td>~ 6.0 +, ~ 5.3 –</td></tr></table>	Casting method	d_c (cm)	Poured, clear	$3.17 < d_c$	Creamed	$2.20 < d_c < 2.54$	Creamed plus 10% fines	$1.26 < d_c < 1.66$	T ($^\circ\text{C}$)	d_c (cm)	–193	10 +, ~ 10.5 +, ~ 9.1 –, ~ 9.4 –, ~ 9.7 –	~ 30	~ 6.5 +, ~ 6.1 +, ~ 6.0 –	75	~ 6.0 +, ~ 5.3 –
Casting method	d_c (cm)																
Poured, clear	$3.17 < d_c$																
Creamed	$2.20 < d_c < 2.54$																
Creamed plus 10% fines	$1.26 < d_c < 1.66$																
T ($^\circ\text{C}$)	d_c (cm)																
–193	10 +, ~ 10.5 +, ~ 9.1 –, ~ 9.4 –, ~ 9.7 –																
~ 30	~ 6.5 +, ~ 6.1 +, ~ 6.0 –																
75	~ 6.0 +, ~ 5.3 –																

Detonation failure limit curves^[70]:

Particle size (μ)	d_c (mm)	% TMD	Particle size (μ)	d_c (mm)	% TMD
10–50	~ 4.5	54	70–200	~ 10	56
10–50	~ 4.0	58	70–200	~ 9	61
10–50	~ 3.5	63	70–200	~ 8	66
10–50	~ 3.0	68	70–200	~ 7	71
			70–200	~ 6	76
			70–200	~ 5	82
			70–200	~ 4	87
			70–200	~ 3	93

Failure diameter = 0.25 cm^[104]

Critical diameters of various forms of TNT, values from^[143]:

Form of charges	ρ_0 , g/cc	% TMD	d_c , mm
Pressed at 25 °C			
ca. 140 μ	1.18	71.5	7.5, 6.4, 7.0
	1.62	98.0	2.0, 1.8, 2.5
ca. 30 μ	1.18	71.5	2.5
	1.60	97.0	ca. 2.5
Pressed at 62–76 °C	1.64	99.2	7.8
Castings			
Poured	Cooling rate		
Clear	Rapid	1.62	98.0 14
Creamed	Moderate	1.61	97.5 24, 27
Clear	Moderate	1.62	98.0 30
Clear	Very slow	1.61	97.5 > 38
Perfect single crystal		1.65	100 –

	<p>Shock sensitivity and detonability of TNT; * higher P on crystal than on liquid is necessary to reach same shocked temperature. This takes into account the lower initial temperature, lower compressibility and lower specific heat of the crystal; † It is assumed that single crystal will have $d_c \geq$ than that of any casting and also that the confinement of the gap test produces an effective diameter of about 76 mm. A special TNT casting was prepared with very slow cooling of the melt. This casting was not detonable in the gap test. Hence the estimate for single crystal TNT^[151]:</p> <table><tr><th>Description</th><th>P (kbar)</th><th>d_c (mm)</th></tr><tr><td>Pressed 70–200 μ, 65% TMD, 25 °C</td><td>10</td><td>8</td></tr><tr><td>Pressed 70–200 μ, 99% TMD, 25 °C</td><td>23</td><td>< 2</td></tr><tr><td>Cast, 25 °C</td><td>26–46</td><td>27 – > 32</td></tr><tr><td>Liquid, 81–83 °C</td><td>~ 110</td><td>68</td></tr><tr><td>Single crystal, 25 °C</td><td>> 110*</td><td>> 76†</td></tr></table> <p>TNT @ 81–83 °C, $\rho_0 = 1.47$ g/cc, $P_i = \sim 110$ kbar, $d_c = 68$ mm^[151], 60 mm @ 100 °C (liq.)^[164]</p> <p>Data from^[170]:</p> <table><tr><th>HE</th><th>Particle size (μ)</th><th>ρ_0</th><th>Approx. d_c (mm)</th></tr><tr><td>TNT</td><td>20–70</td><td>1.60</td><td>3.25</td></tr><tr><td>TNT</td><td>400–800</td><td>1.57</td><td>3.30</td></tr></table> <p>Detonation failure thickness values^[25]:</p> <table><tr><th>Density (g/cm³)</th><th>Failure thickness (mm)</th><th>Remarks</th></tr><tr><td>1.568</td><td>1.82</td><td>Pressed @ 65 °C</td></tr><tr><td>1.627</td><td>2.16</td><td>Pressed @ 65 °C</td></tr><tr><td>1.629</td><td>1.76</td><td>Pressed @ 65 °C</td></tr><tr><td>1.631</td><td>2.00</td><td>Pressed @ 72 °C</td></tr><tr><td>1.635</td><td>2.59</td><td>Pressed @ 72 °C</td></tr></table>	Description	P (kbar)	d_c (mm)	Pressed 70–200 μ , 65% TMD, 25 °C	10	8	Pressed 70–200 μ , 99% TMD, 25 °C	23	< 2	Cast, 25 °C	26–46	27 – > 32	Liquid, 81–83 °C	~ 110	68	Single crystal, 25 °C	> 110*	> 76†	HE	Particle size (μ)	ρ_0	Approx. d_c (mm)	TNT	20–70	1.60	3.25	TNT	400–800	1.57	3.30	Density (g/cm ³)	Failure thickness (mm)	Remarks	1.568	1.82	Pressed @ 65 °C	1.627	2.16	Pressed @ 65 °C	1.629	1.76	Pressed @ 65 °C	1.631	2.00	Pressed @ 72 °C	1.635	2.59	Pressed @ 72 °C
Description	P (kbar)	d_c (mm)																																															
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Failure diameter	1 in ^[165]																																																
Critical pressures of explosion initiation [GPa]	$P_{cr} = \sim 1.1$ (TNT, impact) ^[119] , $\sigma_{ult} = 36$ MPa (TNT, impact) ^[119] , $P_{cr} = 1.30 \pm 0.03$ (TNT, DT) ^[119] , $P_{cr} = 1.08 \pm 0.03$ (recryst. TNT, impact) ^[119] , $\sigma_{ult} = 39$ MPa (recryst. TNT, impact) ^[119] , $P_{cr} = 1.27 \pm 0.03$ (recryst. TNT, DT) ^[119] , $P_{cr} = 1.40$ ^[134] , $\sigma_{ult} = 47$ MPa ^[134]																																																
Critical T [°C]	287–289 (exptl.) ^[125, 141] , 291 (calcd.) ^[125, 141] , 970 K (explosion in 250 ms) ^[161] , 288 (T_m) ^[25]																																																

Trauzl test [cm ³ , % TNT]	TNT = standard, 100% ^[23] , 285–305 cm ³ (10 g TNT) ^[27] , 90–95% PA ^[43] , 285–300 cc ^[44] , 260–310 cm ³ (i.e. 94–98% PA) ^[88] , 452 cc (15 g sample) ^[93] , 12.2 cc (small Trauzl test) ^[89, 145] , 285 cm ³ (10 g sample, sand tamping) ^[89] , 60% PETN ^[89] , 285 cc ^[163, 172] , 1.07 (cycled TNT) cf. TNT as 1.00 ^[167] , 300 ^[172] , 303 ^[172] , 310 ^[172]												
Lead block test	14.8 mm shortening (small lead block compression test, 50 g TNT, exploded by detonator on top of lead cylinder 64 mm long) ^[89]												
Sand test [g]	48.0 g (200 g bomb) ^[17, 23] , 41.2 g sand crushed (1,700 g bomb, 0.4 g sample) ^[43] , 48.0 g sand crushed ^[33] , 95% PA ^[88] , 55.3 g (amount of sand crushed finer than 30 mesh, by total charge consisting of base charge of 0.50 g TNT and 0.30 g priming charge of MF) ^[145] , 43.6 g (amount of sand crushed finer than 30 mesh, by base charge of 0.50 g TNT) ^[145]												
Ballistic mortar test	TNT = standard, 100% ^[23] , 90% PA ^[88]												
Initiation efficiency	<p>Dry TNT can be detonated by No. 6 electric blasting cap^[27], 7% moisture prevents detonation by No. 6 electric blasting cap^[27]</p> <p>Minimum charges of fulminate:chlorate (90:10) necessary to cause detonation of TNT and TNT/Tetryl mixtures^[93]:</p> <table><tr><td>TNT-Tetryl</td><td>Weight of initiator (g)</td><td>TNT-Tetryl</td><td>Weight of initiator (g)</td></tr><tr><td>100–0</td><td>0.25</td><td>80–20</td><td>0.21</td></tr><tr><td>90–10</td><td>0.22</td><td>50–50</td><td>0.20</td></tr></table> <p>Amount of azides or fulminates necessary to cause detonation of TNT^[89]: 0.04 g cadmium azide^[89], 0.07 g silver azide^[89], 0.09 g LA^[89], 0.095 g cuprous azide^[89], 0.145 g mercurous azide^[89], 0.335 g thallium azide^[89], 0.095 g silver fulminate^[89], 0.11 g cadmium fulminate^[89], 0.15 g copper fulminate^[89], 0.36 g mercury fulminate^[89], minimum detonating charge of LA = 0.27 g^[165]</p> <p>Minimum initiating charge (g) of primary explosive necessary to cause detonation of 0.4 g TNT (TNT and primary explosive compressed in detonator capsule under 1,000 lb/in²): 0.26 g fulminate (with reinforcing cap)^[89], 0.08 g HMTD (with reinforcing cap)^[89], 0.10 g HMTD (without reinforcing cap)^[89]</p> <p>Minimum initiating charge of primary explosive necessary to cause detonation (0.4 g TNT loaded into detonator capsule, pressed down, initiator added, covered with short reinforcing cap, pressed with 200 atm./in²)^[89]: 0.10 g cyanuric azide^[89], 0.26 g mercury fulminate^[89]</p>	TNT-Tetryl	Weight of initiator (g)	TNT-Tetryl	Weight of initiator (g)	100–0	0.25	80–20	0.21	90–10	0.22	50–50	0.20
TNT-Tetryl	Weight of initiator (g)	TNT-Tetryl	Weight of initiator (g)										
100–0	0.25	80–20	0.21										
90–10	0.22	50–50	0.20										

	<p>Minimum initiating charge of primary explosive necessary to cause detonation (0.5 g TNT loaded into No. 8 detonator capsule, with reinforcing cap, pressed with 3,400 lb/in²): 0.240 g MF^[89], 0.163 g DDNP^[89], 0.16 g LA^[89]</p> <p>Can be detonated by No. 6 blasting cap if in crystalline or granular form^[142], can be detonated by No. 8 blasting cap if in highly pressed form^[142], booster required for consistent detonation if in cast form^[142], can be detonated by No 6 electric blasting cap^[149]</p> <p>Minimum weight of priming charge which causes complete detonation of the base charge^[145]: 0.163 g DDNP^[145], 0.240 g MF^[145], 0.16 g LA^[145]</p> <p>Limit of initiation charge of MF for TNT = 0.36 g^[163], cast TNT is less sensitive to detonation^[163], cannot be detonated by No. 8 detonating cap^[163]</p> <p>0.27 minimum detonating charge of LA required to shock initiate TNT^[181], 270 mg dextrinated LA required^[183], 70 mg silver azide required^[183]</p>																						
US NOL gap test	<p>Gap thickness = 4.90 cm @ 1.569 g cm⁻³ (pressed TNT)^[28, 91] Gap thickness = 3.50 cm @ 1.60 g cm⁻³ (cast TNT)^[28, 91] 34 mm (133 cards) (cast TNT, 50% probability point)^[84] 45 mm (175 cards) (pressed TNT, 50% probability point)^[84]</p> <p>Confined/unconfined NOL LSGT / TNT-c = cast TNT)^[69]:</p> <table><tr><th rowspan="2">Material</th><th rowspan="2">ρ_0 (g cm⁻³)</th><th colspan="2">50% gap (in. × 10²)</th></tr><tr><th>Confined</th><th>Unconfined</th></tr><tr><td>TNT-c</td><td>1.61–1.62</td><td>135</td><td>73</td></tr></table> <p>Comparison of NOL LSGT results with those of IHE gap test, TNT-c = cast TNT, TNT-p = pressed TNT^[69]:</p> <table><tr><th>Material</th><th>ρ_0 (g cm⁻³)</th><th>IHE (50% gap, in.)</th><th>LSGT (in × 10²)</th></tr><tr><td>TNT-c</td><td>1.61</td><td>1.30</td><td>124–135</td></tr><tr><td>TNT-p</td><td>1.57</td><td>1.92</td><td>193–198</td></tr></table>	Material	ρ_0 (g cm ⁻³)	50% gap (in. × 10 ²)		Confined	Unconfined	TNT-c	1.61–1.62	135	73	Material	ρ_0 (g cm ⁻³)	IHE (50% gap, in.)	LSGT (in × 10 ²)	TNT-c	1.61	1.30	124–135	TNT-p	1.57	1.92	193–198
Material	ρ_0 (g cm ⁻³)			50% gap (in. × 10 ²)																			
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LSGT shock sensitivity data for various forms of TNT; values in parenthesis were not measured; * tested at $d = 5.08$ cm because $d_c = 3.81$ cm; † = vacuum cast; ‡ = estimate; § = entering shock at zero gap induced fading reaction. Front travelled at 6.8 mm/s for 5–6 cm and then at 4.7 mm/s for next 9–10 cm; # = only one shot at zero gap, measured detonation velocity was 6.9 mm/s [143];													
Form of charges		ρ_0 (g/cc) % TMD		Unconfined (d = 3.81 cm)				Confined ($d_c \sim 7.6$ cm)				d/d_c	
				50% point				50% point					
				Gap (mm)	P_k (kbar)	P_l (kbar)	Gap (mm)	P_k (kbar)	P_l (kbar)	Gap (mm)			
Pressed at 25 °C		1.18	71.5	(50.3	18	13)		63.7	11	8		10	
		1.62	98.0	(29.7	43	49)		45.2	22	25		35	
Castings													
Poured	Cooling rate												
Clear	Rapid	1.57	95.0	24.9	50	61		(40.2	28	32)		5	
Creamed	Moderate	1.615	97.75	18.5	62	74		34.3	37	43		3	
Clear†	Moderate	1.62	98.0	9.7*	87.5*	104*		(20.6	58	69)		3	
Clear	Very slow	1.61	97.5	Subcritical[§				> 0#					
Perfect single crystal		1.65	100	-						> 125#		3	

	<p>^a = relationship $P_i = a + b d^{-1}$ assumed (TNT Hugoniot was used for DINA), ^b = standard LSGT confined charge assumed equivalent to 7.62 cm diameter unconfined charge^[170]:</p> <table><tr><th rowspan="2">ρ_0 (g cm⁻³)</th><th rowspan="2">d_e (cm)</th><th colspan="3">50% point</th><th>Slope^a</th></tr><tr><th>Gap (in × 10²)</th><th>P_g (kbar)</th><th>P_i (kbar)</th><th>$\Delta P/\Delta d^{-1}$ (kbar-cm)</th></tr><tr><td>1.62</td><td>3.81</td><td>73</td><td>66.2</td><td>79.5</td><td rowspan="2">210</td></tr><tr><td>1.61</td><td>7.62^b</td><td>135</td><td>43.9</td><td>52.0</td></tr></table>	ρ_0 (g cm ⁻³)	d_e (cm)	50% point			Slope ^a	Gap (in × 10 ²)	P_g (kbar)	P_i (kbar)	$\Delta P/\Delta d^{-1}$ (kbar-cm)	1.62	3.81	73	66.2	79.5	210	1.61	7.62 ^b	135	43.9	52.0
ρ_0 (g cm ⁻³)	d_e (cm)			50% point			Slope ^a															
		Gap (in × 10 ²)	P_g (kbar)	P_i (kbar)	$\Delta P/\Delta d^{-1}$ (kbar-cm)																	
1.62	3.81	73	66.2	79.5	210																	
1.61	7.62 ^b	135	43.9	52.0																		
Modified gap test	<p>Pressures required to produce burning or detonation in pressed or cast TNT using the modified gap test^[33]:</p> <table><tr><th>TNT</th><th>Burning^[33]</th><th>Detonation^[33]</th></tr><tr><td>Pressed</td><td>22 kb</td><td>50 kb</td></tr><tr><td>Cast</td><td>22 kb</td><td>90 kb (by extrapolating)</td></tr></table>	TNT	Burning ^[33]	Detonation ^[33]	Pressed	22 kb	50 kb	Cast	22 kb	90 kb (by extrapolating)												
TNT	Burning ^[33]	Detonation ^[33]																				
Pressed	22 kb	50 kb																				
Cast	22 kb	90 kb (by extrapolating)																				
LASL LSGT ²	<p>TNT-c (cast): $\rho = 1.62$ g cm⁻³, critical diameter = 26.9 mm, LASL LSGT² = 29.30 mm^[57], TNT-creamed cast*: ρ = not given, critical diameter = 23.7 ± 1.7 mm, LASL LSGT² = not given^[57], TNT-p (pressed): $\rho = 1.63$ g cm⁻³, critical diameter = 2.62 mm, LASL LSGT² = 51.79 mm^[57], cast TNT @ 1.615 g cm⁻³, 97.6% TMD, $L_g = 111$ in. × 10²^[70], pressed TNT @ 1.595 g cm⁻³, 96.4% TMD, $L_g = 204$ in. × 10² (pressed @ 25 °C)^[70], pressed TNT @ 1.627 g cm⁻³, 98.4% TMD, $L_g = 194$ in × 10² (pressed @ 75 °C)^[70], pressed TNT @ 1.637 g cm⁻³, 99.0% TMD, $L_g = 168$ in. × 10² (pressed @ 72 °C)^[70]</p>																					

LSGT [cm]	Shock sensitivity data for various forms of TNT ^[67] :									
	Form of charges	ρ_0 (g cm ⁻³)	% TMD	Unconfined (d = 3.81 cm), 50% point			Confined (d _c ~ 7.6 cm = 50% point			
Pressed @ 25 °C				Gap (mm)	P _g (kbar)	P _i (kbar)	Gap (mm)	P _g (kbar)	P _i (kbar)	d _e /d _c
		1.18	71.5	50.3 ^b	18 ^b	13 ^b	63.7	11	8	10
Perfect single crystal		1.62	98.0	29.7 ^b	43 ^b	49 ^b	45.2	22	25	35
		1.65	100	-	-	-	-	-	> 125 ^f	3
Castings										
Poured/cooling rate										
Clear/rapid	1.57	95.0		24.9	50	61	40.2 ^b	28 ^b	32 ^b	5
Creamed/moderate	1.615	97.75		18.5	62	74	34.3	37	43	3
Clear ^a /moderate	1.62	98.0		9.7 ^c	87.5 ^c	104 ^c	20.6 ^b	58 ^b	69 ^b	3
Clear/very slow	1.61	97.5		Subcritical			> 0 ^e			

^a = vacuum cast, ^b = not measured values, ^c = tested @ d = 5.08 cm because d_c = 3.81 cm, ^e = only 1 shot @ zero gap, measured VoD = 6.9 mm/μs, ^f = est. value^[67]

46 mm (pressed TNT, NOL)^[85], 30 mm (pressed TNT, LANL)^[85], 30 (cast TNT, NOL)^[85], 27 (cast TNT, LANL)^[85]

Cast TNT , NSWC @ 1.61 g cm⁻³, 97.3% TMD, $L_g = 133 \text{ in} \times 10^{2[70]}$, Pressed TNT @ 1.60 g cm⁻³, 97.1% TMD, $L_g = 183 \text{ in} \times 10^{2[70]}$, Pressed TNT @ 1.64 g cm⁻³, 99.0% TMD, $L_g = 175 \text{ in} \times 10^2$ (isostatically pressed; water @ 88 °C)^[70], $G_{50} = 21.86 \text{ mm}^{[124]}$

Gap test results for TNT^[27]:

	Density (g/cc)	% Voids	Sensitivity (mm)
LANL LSGT	0.87 (flake)	47.4	37.1
	0.73 (granular)	55.9	60.8

Pressed TNT @ 1.58 g cm⁻³ (96% TMD), gap material = Ly-12A1, $G_{50} = 42.5 \text{ mm}^{[157]}$, no positive test @ 50 cards for a slurry of TNT and DMF containing a 50% excess of TNT cf. the amount of TNT required to give a saturated soln. in DMF @ 25 °C (NOL LSGT)^[160], 282 cards (TNT @ 65% TMD, NOL LSGT)^[160], 224 cards (TNT @ 80.6% TMD, NOL LSGT)^[160], 193 cards (TNT @ 95.7% TMD, NOL LSGT)^[160], 133 cards (TNT @ 96.6% TMD, NOL LSGT)^[160], cast TNT, TMD = 1.654 g cm⁻³, expt. $\rho = 1.62 \text{ g cm}^{-3}$, 98.1% TMD, gap = 108 cards (only one cast TNT in the literature showed a value below 120 cards)^[169], $\rho_0 = 1.35 \text{ g/cc}$, 81.8% TMD, 50% pressure (P_g) = 14.9 kbar (interpolated)^[170], critical initiating pressure (P_i) from LSGT^[170]: $\rho_0 = \sim 1.60 \text{ g/cc}$, 50% point = 133 cards, $P_g = 44.4 \text{ kbar}$, critical pressure, $P_i = 52.7 \text{ kbar}$, TNT Hugoniot used^[170]

Data from^[170]:

Density		50% point		Particle size (µm)	Remarks
g/cm ³	% TMD	Cards	kbar		
1.07P	65.0	262	10		
1.25H	75.8	239	14		
1.32I	80.2	234	15	200	Coarse TNT (retained on 200 mesh screen)
1.33I	80.4	231	15	100	Fine TNT (through 200 mesh screen)
1.33H	80.6	224	(16)		Granular TNT from Yorktown
1.42I	85.8	213	17		
1.49I	90.5	208	18		

1.58I	95.7	193	(22)		Granular TNT from Yorktown
1.58I	95.7	198	20		Granular TNT from Dupont
1.60I	97.1	183	24		
1.64I	99.0	175	26		Water heated to 88 °C during pressing; no evidence of melting on surface of charge; density varied between 1.63 and 1.64
1.62C	98.1	124	47		
1.61C	97.5	124	47		Repacked
1.60C	97.1	162	31		Repacked, difference from test above attributed to difference in casting or in sample taken from different box of this lot
1.61C	97.3	133	(44)		Granular TNT from Yorktown
1.61C	97.3	135	44		Flake TNT from Yorktown
1.62C	98.1	73	66		Flake TNT from Yorktown, unconfined
1.58C	96.0	145	39		Granular TNT from Holston, recryst.
1.59C	96.6	133	44		Granular TNT from DuPont
1.62C	98.1	108E	52		
1.62C	98.1	121	48		Granular TNT from DuPont, cast Pentolite witness
1.56C	94.8	96	57		Stand cast, 2 in diam. bare charges, for Dahlgren
1.56C	94.8	98	56		Stand cast, 1-1/2 in diam bare charges, for Dahlgren
1.62C	98.1	38	88		Vac cast, 2 in diam. bare charges, for Dahlgren
1.62C	98.1	47	81		Vac cast, 1-1/2 in diam. bare charges

	<p>C = cast, I = isostatic press, H = hydraulic press, p = packed by hand; at 0 card gap X, G and Q indicate no go, go and questionable (X = flat plate, G = hole in plate and Q = plate damage but no hole); type of test = regular unless listed as E (extended) or M (modified); all charges are conditioned and fired at 25 °C except where noted.</p> <p>Data from^[25]:</p> <table><tr><th>Density (g/cm³)</th><th>G₅₀ (mm)</th><th>L₉₅ (mm)</th><th>Remarks</th></tr><tr><td colspan="4">Large scale</td></tr><tr><td>0.800</td><td>61.49</td><td>0.38</td><td>Bulk density flake</td></tr><tr><td>1.024</td><td>61.54</td><td>0.20</td><td>Pressed</td></tr><tr><td>1.220</td><td>56.26</td><td>0.08</td><td>Pressed</td></tr><tr><td>1.356</td><td>55.02</td><td>0.25</td><td>Pressed</td></tr><tr><td>1.505</td><td>54.92</td><td>0.30</td><td>Pressed</td></tr><tr><td>1.551</td><td>54.46</td><td>0.28</td><td>Pressed</td></tr><tr><td>1.595</td><td>52.53</td><td>0.18</td><td>Pressed</td></tr><tr><td>1.631</td><td>46.43</td><td>0.30</td><td>Pressed</td></tr><tr><td>1.615</td><td>28.30</td><td>0.64</td><td>Cast</td></tr></table>	Density (g/cm ³)	G ₅₀ (mm)	L ₉₅ (mm)	Remarks	Large scale				0.800	61.49	0.38	Bulk density flake	1.024	61.54	0.20	Pressed	1.220	56.26	0.08	Pressed	1.356	55.02	0.25	Pressed	1.505	54.92	0.30	Pressed	1.551	54.46	0.28	Pressed	1.595	52.53	0.18	Pressed	1.631	46.43	0.30	Pressed	1.615	28.30	0.64	Cast
Density (g/cm ³)	G ₅₀ (mm)	L ₉₅ (mm)	Remarks																																										
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SSGT [cm]	<p>Gap test results for TNT^[27]:</p> <table><tr><th></th><th>Density (g/cc)</th><th>% Voids</th><th>Sensitivity (mm)</th></tr><tr><td rowspan="3">NSWC SSGT</td><td>1.651</td><td>0</td><td>3.96</td></tr><tr><td>1.561</td><td>5.5</td><td>6.25</td></tr><tr><td>1.353</td><td>18.0</td><td>7.90</td></tr><tr><td rowspan="3">LANL SSGT</td><td>1.633</td><td>1.3</td><td>0.33</td></tr><tr><td>0.84</td><td>49.2</td><td>No go</td></tr><tr><td>0.77</td><td>53.4</td><td>4.11</td></tr></table>		Density (g/cc)	% Voids	Sensitivity (mm)	NSWC SSGT	1.651	0	3.96	1.561	5.5	6.25	1.353	18.0	7.90	LANL SSGT	1.633	1.3	0.33	0.84	49.2	No go	0.77	53.4	4.11																				
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Data from^[25]:

Small scale*			
0.77	4.11	0.08	Granular at bulk density
0.84	No go at zero gap		Flake at bulk density
1.628	0.33	0.05	Pressed @ 65 °C

*The failure diameter of cast TNT is 14.5 mm, so it cannot be initiated in the small-scale gap test

Underwater: critical length, $L_c = 6$ mm^[29, 86], 5.7 mm (pressed TNT, NOL)^[85], 0.4 mm (pressed TNT, LANL)^[85], $G_{50} = 5.66$ mm^[124]

Small-scale gap (booster) sensitivity test (pressed TNT)^[96]:

@ 93% TMD		@ 95% TMD	
DBg	Lucite gap (mils)	DBg	Lucite gap (mils)
5.7	269	60	251

DBg = 30–10 log (test gap/ref. gap)^[96]

$P_{90} = 17.72$ kbar (P_{90} = pressure to 90% of TMD, NSWC small-scale gap test)^[107]

TNT, TMD = 1.651 g cm⁻³, data from^[168]:

Loading pressure (kpsi)	Density (g/cm ³)		% TMD	Sensitivity (DBG)			
	AVG.	s		AVG.	g	s_m	N
7.0	1.413	0.0041	85.6	5.255	0.0237	0.0107	46
11.0	1.489	0.0068	90.2	5.523	0.1428	0.0493	46
19.0	1.568	0.0039	95.0	6.130	0.0429	0.0176	46

	<p>TNT, TMD = 1.651 g cm⁻³, data from^[168]:</p> <table><tr><th rowspan="2">Loading pressure (kpsi)</th><th colspan="2">Density (g/cm³)</th><th rowspan="2">% TMD</th><th colspan="4">Sensitivity (DBG)</th></tr><tr><th>AVG.</th><th><i>s</i></th><th>AVG.</th><th><i>g</i></th><th><i>s_m</i></th><th><i>N</i></th></tr><tr><td>4</td><td>1.353</td><td>0.0130</td><td>82.0</td><td>5.067</td><td>0.0321</td><td>0.0274</td><td>18</td></tr><tr><td>8</td><td>1.446</td><td>0.0079</td><td>87.6</td><td>5.316</td><td>0.0338</td><td>0.0277</td><td>18</td></tr><tr><td>16</td><td>1.549</td><td>0.0024</td><td>93.8</td><td>5.877</td><td>0.0645</td><td>0.0366</td><td>18</td></tr><tr><td>32</td><td>1.623</td><td>0.0019</td><td>98.3</td><td>6.703</td><td>0.0434</td><td>0.0321</td><td>18</td></tr><tr><td>64</td><td>1.651</td><td>0.0025</td><td>100.0</td><td>8.066</td><td>0.0710</td><td>0.0446</td><td>18</td></tr></table> <p>TNT, TMD = 1.651 g cm⁻³, data from^[168]:</p> <table><tr><th rowspan="2">Loading pressure (kpsi)</th><th colspan="2">Density (g/cm³)</th><th rowspan="2">% TMD</th><th colspan="4">Sensitivity (DBG)</th></tr><tr><th>AVG.</th><th><i>s</i></th><th>AVG.</th><th><i>g</i></th><th><i>s_m</i></th><th><i>N</i></th></tr><tr><td>6.2</td><td>1.386</td><td>0.0066</td><td>83.9</td><td>4.551</td><td>0.0495</td><td>0.0317</td><td>53</td></tr><tr><td>19</td><td>1.561</td><td>0.0064</td><td>94.5</td><td>6.095</td><td>0.1186</td><td>0.0539</td><td>42</td></tr></table> <p>ρ_0 = 1.35 g/cc, 81.8% TMD, 50% pressure (P_g) = 17.5 kbar^[170]</p>	Loading pressure (kpsi)	Density (g/cm ³)		% TMD	Sensitivity (DBG)				AVG.	<i>s</i>	AVG.	<i>g</i>	<i>s_m</i>	<i>N</i>	4	1.353	0.0130	82.0	5.067	0.0321	0.0274	18	8	1.446	0.0079	87.6	5.316	0.0338	0.0277	18	16	1.549	0.0024	93.8	5.877	0.0645	0.0366	18	32	1.623	0.0019	98.3	6.703	0.0434	0.0321	18	64	1.651	0.0025	100.0	8.066	0.0710	0.0446	18	Loading pressure (kpsi)	Density (g/cm ³)		% TMD	Sensitivity (DBG)				AVG.	<i>s</i>	AVG.	<i>g</i>	<i>s_m</i>	<i>N</i>	6.2	1.386	0.0066	83.9	4.551	0.0495	0.0317	53	19	1.561	0.0064	94.5	6.095	0.1186	0.0539	42
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Gap test	<p>Comparison of values from gap tests and steel bullet tests^[66]</p> <table><tr><th rowspan="2">Material</th><th colspan="2">From gap test</th><th colspan="2">Velocity for 0.5 in diameter projectiles</th></tr><tr><th>Initial pressure (kbar)</th><th>Cyl. vol. (ft/s)</th><th>Cylinders (ft/s)</th><th>Spheres (ft/s)</th></tr><tr><td>Cast TNT</td><td>37.3</td><td>2,296</td><td>3,720 (est.)</td><td>6,924</td></tr><tr><td>Pressed TNT (ρ = 1.32 g cm⁻³)</td><td>(14.7)</td><td>(1,050)</td><td>2,346 (est.)</td><td>2,913</td></tr></table> <p>Low impulse reactions^[66]:</p> <table><tr><th>Material</th><th>Witness system</th><th>50% Gap (no. cards)</th><th>Initiating pressure (kbar)</th></tr><tr><td>TNT</td><td>Steel plate</td><td>141 ± 1</td><td>36.7</td></tr></table>	Material	From gap test		Velocity for 0.5 in diameter projectiles		Initial pressure (kbar)	Cyl. vol. (ft/s)	Cylinders (ft/s)	Spheres (ft/s)	Cast TNT	37.3	2,296	3,720 (est.)	6,924	Pressed TNT (ρ = 1.32 g cm ⁻³)	(14.7)	(1,050)	2,346 (est.)	2,913	Material	Witness system	50% Gap (no. cards)	Initiating pressure (kbar)	TNT	Steel plate	141 ± 1	36.7																																																									
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	<p>LSGT results for cast TNT ($\rho = 1.62 \text{ g cm}^{-3}$), 50% values, both values corrected to pentolite donor^[69]: NOL LSGT L, cards = 129, LANL LSGT L = 29.30 mm^[69] Gap = 61 mm (detonation), Gap = 62 mm (no detonation)^[72], Gap test $\geq 50 \text{ kbar}$ (cast)^[98]</p> <p>Scale I (detonator = standard commercial No. 8 Briska type, donor = $2 \times 20 \text{ g}$ pellets of Tetryl pressed to $\rho = 1.5 \text{ g/ml}$, each 10 g in weight, gap = stack of cards, 3 in square and 0.050 in thick, charge case = 6 in length of mild steel electrical conduit of 27 mm inner diameter and 31 mm outer diameter, faced end is sealed with Durofix cement, cast TNT) critical card value = 9^[159]</p>						
5 s explosion $T [^{\circ}\text{C}]$ Explosion $T [^{\circ}\text{C}]$	<p>300–310^[28], 475^[23, 149], 475 (dec., cook-off)^[165], 475 (dec.)^[181]</p> <p>570 (0.1 s, no cap used)^[23], 520 (1 s)^[23, 165], 465 (10 s)^[23], 240^[43], 321 (bath heating rate @ 20°C/min)^[30], 304 (bath heating rate @ 5°C/min)^[30], 346 (after 42.5 s)^[33], 430 (after 14.5 s)^[33], 328 (50 s., 50 mg sample)^[33], 475 (unconfined TNT)^[27], 275–295 (depends on sample purity)^[27], 320–325 (closed glass capillary tube)^[27], 570 (0.1 s)^[165], 465 (dec., 10 s)^[165]</p>						
5 s ignition $T [^{\circ}\text{C}]$	475 (dec., USA value) ^[28, 123, 165] , 310, 475 (dec.) (Russian values) ^[28]						
Ignition $T [^{\circ}\text{C}]$	248 (11.55 minutes heating time after bath reached 100°C) ^[44] , 276 (19.87 minutes heating time after bath reached 100°C) ^[44] , 284 (39.58 minutes heating time after bath reached 100°C) ^[44] , 200 (~38 h, autoignition) ^[33] , 240 ^[91] , 277 (calorimetric measurement) ^[123] , 295–300 ^[123]						
Ignition/ Explosion $T [^{\circ}\text{C}]$	<p>Confined samples: 275, 295, 287–289^[33], 295–300^[89] Unconfined samples: 475^[33] Heating in closed glass capillary: 320–335^[33] TNT is difficult to ignite, if directly heated in flame melting occurs; ignition occurs only at high temperature ($T \sim 300^{\circ}\text{C}$)^[88] True ignition @ 295–330 (<i>Kast</i>)^[88], true ignition @ 281–286 (<i>Verola</i>)^[88], true ignition @ 312–316 (<i>Micewicz</i>)^[88], TNT ignites in 30 min @ 240°C (<i>Kast</i>)^[88] 321°C (heated from 100°C @ 20°C/min)^[93], 304°C (heated from 100°C @ 5°C/min)^[93] 290 (α-TNT, 2,4,6-TNT)^[88], 302 (β-TNT, 2,3,4-TNT)^[88], 291 (γ-TNT, 2,4,5-TNT)^[88], 313 (δ-TNT, 3,4,5-TNT)^[88], 332 (ϵ-TNT, 2,3,5-TNT)^[88], 335 (ζ-TNT, 2,3,6-TNT)^[88]</p>						
Initiation $T [^{\circ}\text{C}]$	465 (10 s) ^[91] , 520 (1 s) ^[91] , 306 ^[130]						
Deflagration $T [^{\circ}\text{C}]$	225 (determined using 2 lb slabs heated @ 100°C/min on one surface) ^[96]						
Detonation $T [^{\circ}\text{C}]$	465 ^[142]						
Explosion $T [^{\circ}\text{C}]$	<p>Explosion temperature vs TNT initial temperature^[23]:</p> <table border="1"> <tr> <th>TNT temperature, initial ($^{\circ}\text{C}$)</th><th>Explosion temperature ($^{\circ}\text{C}$)</th></tr> <tr> <td>Room</td><td>470 (dec)</td></tr> <tr> <td>105–100</td><td>480 (dec)</td></tr> </table>	TNT temperature, initial ($^{\circ}\text{C}$)	Explosion temperature ($^{\circ}\text{C}$)	Room	470 (dec)	105–100	480 (dec)
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	Explosion temperature vs confinement ^{t[23]} : <table><tr><td>Confinement</td><td>Explosion temperature (°C)</td></tr><tr><td>Unconfined</td><td>470 (dec)</td></tr><tr><td>Sealed in glass capillary</td><td>320–335 (explodes)</td></tr></table>	Confinement	Explosion temperature (°C)	Unconfined	470 (dec)	Sealed in glass capillary	320–335 (explodes)			
Confinement	Explosion temperature (°C)									
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Autoignition T [°C]	After 38 h @ 200 °C ^[27]									
100 °C heat test [% mass loss]	0.2% loss in first 48 h ^[23] , 0.2% loss in second 48 h ^[23] , no explosions in 100 h ^[23]									
75 °C Int. heat test	0.04% loss in 48 h ^[23]									
Vacuum stability test [cm ³ /h]	0.10 cc/40 h @ 100 °C ^[23] , 0.23 cc/40 h @ 120 °C ^[23, 165] , 0.44 cc/40 h @ 135 °C ^[23] , 0.65 cc/40 h @ 150 °C ^[23] , 0.2 mL/g gas evolved after 48 h @ 120 °C ^[25] , 0.1 cm ³ /g/48 h @ 100 °C ^[33] , 0.01 cm ³ @ 110 °C/20 h (ρ TNT = 1.65 g cm ⁻³) ^[78, 115, 122] , <0.1 cc/g/48 h @ 100 °C ^[96, 104] , 0.3 mL/5 g @ 120 °C, 48 h ^[124] , @ 175 °C: 8.0 cm ³ /2 days, 45.0 cm ³ /7 days ^[52] , @ 150 °C: 0.3 cm ³ /2 days, 0.7 cm ³ /7 days, 1.3 cm ³ /14 days, 2.7 cm ³ /21 days, 7.0 cm ³ /28 days, 18.1 cm ³ /35 days ^[52] , 0.23 mL after 40 h @ 120 °C ^[181]									
Thermal stability	<p>TNT pellets pressed from flakes show substantial decrease in rate of detonation and sensitivity to initiation after storing for 7 days @ 65 °C^[27], no decomposition after 20 years storage in a magazine^[27, 33, 149], no decomposition after storing as a liquid @ 85 °C^[27, 33], TNT vapor shows no decomposition between 250 and 301 °C @ 35–500 mm Hg^[33], small amount of dec. after 40 h @ 150 °C^[27], slow dec. occurs >150 °C^[27], TNT vapor undergoes dec. @ 250–301 °C @ 35–500 Torr^[27], extensive dec. @ 357 °C but no explosion^[27]</p> <p>No. of moles of gas produced per mole TNT/no. h^[47]: @ 120 °C: 0/22, 0/72^[47], @ 220 °C: 1.83/22, 2.18/72^[47], @ 120 °C: 2.68/22, 3.23/72^[47]</p> <p>No dec. after heating @ 130 °C for 100 h^[88], no gaseous dec. products after heating @ 150 °C for 4 h^[88], gaseous dec. products start being produced @ 160 °C^[88], TNT ignites in 30 min @ 240 °C (<i>Kast</i>)^[88], exothermic dec. @ 270 °C (<i>Kast</i>)^[88], true ignition @ 295–330 (<i>Kast</i>)^[88], true ignition @ 281–286 (<i>Verola</i>)^[88], true ignition @ 312–316 (<i>Micewicz</i>)^[88], slow dec. on heating @ 180–200 °C (gas evolved @ 180 °C but no obvious dec. @ 150 °C)^[93]</p> <p>Values from^[99]:</p> <table><tr><td>Storage time @ 65.5 °C</td><td>K-F value (mass %)</td><td>Mass loss after storage</td></tr><tr><td>None</td><td>0.01</td><td>–</td></tr><tr><td>4 months</td><td>0.09</td><td>0.09%</td></tr></table> <p>0.65% mass loss @ 120 °C, 48 h^[124]</p>	Storage time @ 65.5 °C	K-F value (mass %)	Mass loss after storage	None	0.01	–	4 months	0.09	0.09%
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Thermal conductivity, λ	<div>Thermal conductivity, cal/s/cm/°C^[23]:</div> <table><tr><th>Density (g/cc)</th><th>Thermal conductivity (cal/s/cm/°C)</th></tr><tr><td>1.19</td><td>5.28×10^{-4}</td></tr><tr><td>1.51</td><td>7.12×10^{-4}</td></tr><tr><td>1.54</td><td>5.6×10^{-4}</td></tr><tr><td>1.67</td><td>12.21×10^{-4}</td></tr></table> <div>Thermal conductivity data from^[25]:</div> <table><tr><th>Density (g/cm³)</th><th>Conductivity (cal/s-cm-°C)</th><th>T range (°C)</th></tr><tr><td>1.59</td><td>6.22×10^{-4}</td><td>10 < T < 45</td></tr><tr><td>1.59</td><td>5.89×10^{-4}</td><td>45 < T < 75</td></tr></table> <div>0.00043 @ 125 °C^[88], 4.61×10^{-4} cal/s/cm/°C^[104]</div>	Density (g/cc)	Thermal conductivity (cal/s/cm/°C)	1.19	5.28×10^{-4}	1.51	7.12×10^{-4}	1.54	5.6×10^{-4}	1.67	12.21×10^{-4}	Density (g/cm ³)	Conductivity (cal/s-cm-°C)	T range (°C)	1.59	6.22×10^{-4}	10 < T < 45	1.59	5.89×10^{-4}	45 < T < 75																																													
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Heat capacity [cal/g °C]	<div>Data from^[25]:</div> <table><tr><th colspan="2">Heat capacity @ constant pressure (cal/g-°C)</th><th>T range (°C)</th></tr><tr><td colspan="2">$0.254 + 7.5 \times 10^{-4} T$ (°C)</td><td>17 < T < 67</td></tr><tr><td colspan="2">$0.309 + 5.5 \times 10^{-4} T$ (°C)</td><td>97 < T < 150</td></tr></table> <div>Values within ± 0.015, 30 mg samples^[101]:</div> <table><tr><th>T (°C)</th><th>Flake TNT (uncycled)</th><th>Flake TNT cycled to 150 °C @ 5 °C/min</th><th>Virgin TNT (uncycled)</th><th>Virgin TNT cycled to 150 °C @ 5 °C/min</th></tr><tr><td>20</td><td>0.247</td><td>0.255</td><td>0.270</td><td>0.278</td></tr><tr><td>30</td><td>0.257</td><td>0.266</td><td>0.280</td><td>0.290</td></tr><tr><td>40</td><td>0.265</td><td>0.274</td><td>0.289</td><td>0.299</td></tr><tr><td>50</td><td>0.276</td><td>0.286</td><td>0.300</td><td>0.311</td></tr><tr><td>60</td><td>0.286</td><td>0.296</td><td>0.311</td><td>0.321</td></tr><tr><td>120</td><td>0.359</td><td>0.372</td><td>0.386</td><td>0.392</td></tr><tr><td>130</td><td>0.361</td><td>0.374</td><td>0.388</td><td>0.395</td></tr><tr><td>140</td><td>0.367</td><td>0.381</td><td>0.396</td><td>0.402</td></tr><tr><td>150</td><td>0.369</td><td>0.384</td><td>0.398</td><td>0.404</td></tr><tr><td>160</td><td>0.375</td><td>0.387</td><td>0.405</td><td>0.411</td></tr></table>	Heat capacity @ constant pressure (cal/g-°C)		T range (°C)	$0.254 + 7.5 \times 10^{-4} T$ (°C)		17 < T < 67	$0.309 + 5.5 \times 10^{-4} T$ (°C)		97 < T < 150	T (°C)	Flake TNT (uncycled)	Flake TNT cycled to 150 °C @ 5 °C/min	Virgin TNT (uncycled)	Virgin TNT cycled to 150 °C @ 5 °C/min	20	0.247	0.255	0.270	0.278	30	0.257	0.266	0.280	0.290	40	0.265	0.274	0.289	0.299	50	0.276	0.286	0.300	0.311	60	0.286	0.296	0.311	0.321	120	0.359	0.372	0.386	0.392	130	0.361	0.374	0.388	0.395	140	0.367	0.381	0.396	0.402	150	0.369	0.384	0.398	0.404	160	0.375	0.387	0.405	0.411
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Specific heat [cal/g/°C]	Values from ^[23] :																																						
	<table><tr><th>T (°C)</th><th>Specific heat (cal/g/°C)</th></tr><tr><td>0</td><td>0.309</td></tr><tr><td>20</td><td>0.328</td></tr><tr><td>50</td><td>0.353</td></tr><tr><td>80</td><td>0.374</td></tr></table>				T (°C)	Specific heat (cal/g/°C)	0	0.309	20	0.328	50	0.353	80	0.374																									
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	0.264 ^[104]																																						
	Values from ^[27] :																																						
	<table><tr><th>T (K)</th><th>Specific heat (J/mol/K)</th><th>T (K)</th><th>Specific heat (J/mol/K)</th></tr><tr><td>10</td><td>3.116</td><td>170</td><td>162.84</td></tr><tr><td>30</td><td>32.71</td><td>190</td><td>177.15</td></tr><tr><td>50</td><td>60.41</td><td>210</td><td>191.24</td></tr><tr><td>70</td><td>82.52</td><td>230</td><td>205.09</td></tr><tr><td>90</td><td>101.70</td><td>250</td><td>218.72</td></tr><tr><td>110</td><td>118.76</td><td>270</td><td>232.12</td></tr><tr><td>130</td><td>133.54</td><td>300</td><td>251.80</td></tr><tr><td>150</td><td>148.30</td><td></td><td></td></tr></table>				T (K)	Specific heat (J/mol/K)	T (K)	Specific heat (J/mol/K)	10	3.116	170	162.84	30	32.71	190	177.15	50	60.41	210	191.24	70	82.52	230	205.09	90	101.70	250	218.72	110	118.76	270	232.12	130	133.54	300	251.80	150	148.30	
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Change in specific heat of TNT with temperature ^[162] :																																							
<table><tr><th>T (°C)</th><th>0</th><th>20</th><th>50</th><th>80</th></tr><tr><td>Specific heat (cal/g/°C)</td><td>0.309</td><td>0.328</td><td>0.353</td><td>0.374</td></tr></table>				T (°C)	0	20	50	80	Specific heat (cal/g/°C)	0.309	0.328	0.353	0.374																										
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Vapor pressure [atm. @ °C]	Values from ^[23] :																																						
	<table><tr><th>T (°C)</th><th>Vapor pressure (mm Hg)</th></tr><tr><td>80</td><td>0.042</td></tr><tr><td>85</td><td>0.053</td></tr><tr><td>90</td><td>0.067</td></tr><tr><td>95</td><td>0.085</td></tr><tr><td>100</td><td>0.106</td></tr></table>				T (°C)	Vapor pressure (mm Hg)	80	0.042	85	0.053	90	0.067	95	0.085	100	0.106																							
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Data from^[25]:

T (°C)	Vapor pressure (mm Hg)
60.1	5.43×10^{-4}
78.5	6.44×10^{-3}
80.2	7.16×10^{-3}
82.4	7.96×10^{-3}
99.5	4.07×10^{-2}
110.6	8.26×10^{-2}
131.1	3.48×10^{-1}
141.4	6.21×10^{-1}

6.63×10^{-3} Torr @ 66 °C^[45], 7.7 ppb (measured @ 25 °C)^[58], 9.4 ppb (v/v, calcd. based on exptl. values, @ 25 °C)^[58], 1.1×10^{-6} Torr @ 20 °C^[77], 25 mm Hg @ 183 °C^[88], 5.51×10^{-6} Torr @ 25 °C (est.)^[138], 8.02×10^{-6} Torr @ 25 °C (est.)^[138], 3.7×10^{-6} Torr @ 25 °C^[138], 13 ppb_v (equilibrium vapor pressure @ 300 K)^[147], 4.7×10^5 ppb_v (equilibrium vapor pressure @ 400 K)^[147], 1.99×10^{-6} mm Hg @ 20 °C^[152]

Calculated parameters of TNT adsorbed on the cantilever^[71]:

T (°C)	35	45	55	75
Partial pressure (Torr)	3.221×10^{-5}	1.087×10^{-4}	3.408×10^{-4}	2.750×10^{-3}
Sublimation rate (g/s)	6.1217×10^{-6}	2.461×10^{-4}	4.863×10^{-4}	0.09928

Values by Menzies et al.^[88]:

T (°C)	Vapor pressure (cm Hg)	T (°C)	Vapor pressure (cm Hg)
60.1	5.43×10^{-5}	99.5	4.07×10^{-3}
78.5	6.44×10^{-4}	110.6	8.26×10^{-3}
80.2	7.16×10^{-4}	131.1	3.48×10^{-2}
82.4	7.96×10^{-4}	141.4	6.21×10^{-2}

	Specific vapor pressure of TNT ^[162] : <table><tr><td><i>T</i> (°C)</td><td>85</td><td>100</td><td>190</td><td>245–250</td></tr><tr><td>Vapor pressure (mm Hg)</td><td>0.053</td><td>0.106</td><td>2</td><td>50</td></tr></table> 5.50 × 10 ^{−6} Torr @ 25 °C ^[175] , 2.31 × 10 ^{−3} Torr @ 70 °C ^[175] , 5.77 × 10 ^{−2} Torr @ 100 °C ^[175]	<i>T</i> (°C)	85	100	190	245–250	Vapor pressure (mm Hg)	0.053	0.106	2	50							
<i>T</i> (°C)	85	100	190	245–250														
Vapor pressure (mm Hg)	0.053	0.106	2	50														
Volatility	Zero @ 30 °C ^[23]																	
Heat of sublimation [kJ/mol]	23.2–33.7 kcal/mol ^[27] , 100.2 ^[79] , 113.2 (exptl.) ^[132] , 102.7 (calcd., QSPR) ^[132] , 28.3 kcal/mol (latent heat of sublimation, calcd. from vapor pressure data) ^[25]																	
Heat of evaporation [kJ/mol]	22.7 kcal/mol ^[88] , 17.5 kcal/mol ^[88] , heat of vaporization = 17–22.7 kcal/mol ^[27] , Δ <i>H</i> _{vap} = 114.1 ^[175]																	
Enthalpy of melting [J/g]	93.47 ± 2.01 (7 measurement average) ^[97] , 99.5 ^[97] , 103.2 ^[97] , 98.51 ^[97]																	
Heat of fusion [kJ/mol]	Δ <i>H</i> _{fusion} = 22.34 ^[126] , 23.5 cal/g ^[138] , heat of fusion = 22.34 cal/g ^[23] , 20.2–25.2 cal/g values reported ^[27] , latent heat of fusion = 21.41 cal/g ^[163] , 23.53 cal/g (5.35 kcal/mol, latent heat of fusion) ^[25]																	
Heat of crystallization [kcal/mol]	5.6 ^[163]																	
Burn rate [mm/s]	Burns completely without detonation when ignited in open air ^[27, 149] Mass burning rate of volatile explosives, TNT ^[166] : <table><tr><th rowspan="2">Material</th><th colspan="5"><i>n</i> (g cm^{−2} s^{−1})</th></tr><tr><th>40 atm.</th><th>100 atm.</th><th>200 atm.</th><th>400 atm.</th><th>1,000 atm.</th></tr><tr><td>Trotyl (TNT)</td><td>0.326</td><td>0.756</td><td>1.47</td><td>2.90</td><td>7.20 6.65</td></tr></table> Burn rate and equilibrium combustion temperature ^[166] : <i>T</i> _e = 1,980 K ^[166] , <i>m</i> = 0.756 g cm ^{−2} s ^{−1} (100 atm.) ^[166]	Material	<i>n</i> (g cm ^{−2} s ^{−1})					40 atm.	100 atm.	200 atm.	400 atm.	1,000 atm.	Trotyl (TNT)	0.326	0.756	1.47	2.90	7.20 6.65
Material	<i>n</i> (g cm ^{−2} s ^{−1})																	
	40 atm.	100 atm.	200 atm.	400 atm.	1,000 atm.													
Trotyl (TNT)	0.326	0.756	1.47	2.90	7.20 6.65													

	Dependence of burning rate of volatile explosives on pressure ^[166] :								
	Substance		$\delta = \rho/\rho_{\max}$		Coefficients in formulae			Pressure (atm.)	
					<i>a</i>	<i>B</i>	<i>v</i>		
	Trotyl (TNT), $\rho_{\max} = 1.66 \text{ g/cm}^3$		~ 1.0		0.04	0.00716	1.0	20–950	
					–	0.022	0.75	35–100	
					–	0.007	1.0	100–950	
			0.98		–	0.025	0.77	28–105	
					–	0.0065	1.0	500–4,000	
	Solubility [g/mL]	Solubility of TNT g/100 g solvent (%) ^[23] :							
		Water		Acetone		Benzene		Toluene	
°C		%	°C	%	°C	%	°C	%	
0		0.0100	0	57	0	13	0	28	
20		0.0130	20	109	20	67	20	153	
40		0.0285	40	228	40	180	60	367	
60		0.0675	60	600	60	478	80	> 1,700	
					80	2,000			
Carbon tetrachloride		Ether		Chloroform		Trichloroethylene			
°C		%	°C	%	°C	%	°C	%	
0		0.20	0	1.73	0	6	25	3.5	
0		0.65	20	3.29	20	19	55	60	
40		1.75			40	66			
60		6.90			60	302			
70		17.34							
75									

Pyridine		Methyl acetate		Ethylene dichloride		β-Ethoxyethyl acetate	
°C	%	°C	%	°C	%	°C	%
20	140	20	73	20	34	20	29.5
40	250	40	135	40	123	40	49
60	640	50	280	60	460	50	96
70	1,250						
Tetrachloroethane		Aniline		Isopropyl alcohol		Ethanol	
°C	%	°C	%	°C	%	°C	%
20	18	10	6.1	20	0.76	0	0.62
40	50	30	11.5	40	1.96	20	1.25
50	100	50	29	50	2.95	40	2.85
		70	74			60	8.4
		80	130			70	15
Isobutyl alcohol		Carbon disulfide		Chlorobenzene			
°C	%	°C	%	°C	%		
0	0.20	0	0.14	20	35		
20	0.61	20	0.44	30	51		
40	1.41	40	1.4	40	79		
50	2.35			50	116		

131 mg/L H₂O @ 25 °C^[75], 130 mg/L H₂O @ 20 °C^[77], very low solubility in H₂O^[88], dissolves in conc. H₂SO₄ and conc. HNO₃^[88], very soluble in dil. HNO₃^[88], readily soluble in common organic solvents such as acetone, benzene, toluene^[88], 0.4 parts dissolve in 100 parts CS₂ @ 15 °C^[88], 2.7 parts soluble in 100 parts CS₂ @ 46 °C^[88], all isomers (α-, β-, γ-, δ-, ζ-) are soluble in most common organic solvents^[88], all isomers are insoluble in H₂O^[88], aqueous solubility = 150 mg/L @ 25 °C^[138], soluble in acetone, EtOH, benzene and CCl₄^[142], 0.10 g/L in H₂O @ 25 °C^[144], practically insoluble in water^[149], slightly soluble in Et₂O, CCl₄, CS₂ and EtOH^[149], readily soluble in acetone, CHCl₃, ethylene chloride, benzene, toluene, aniline and other solvents^[149], 130 mg/L H₂O @ 25 °C^[152], 1.5 × 10⁻¹ @ 25 °C^[175]

Solubility of α -TNT in 100 g nitric acid^[88]:

Conc. HNO ₃ (%)	T (°C)	Solubility (g)	Conc. HNO ₃ (%)	T (°C)	Solubility (g)
78.2	48	100	84.7	33	100
	53	150		41	150
	56	200		46	200
	59	250		54	300
	61	300			
80.4	44	100	91.8	26	150
	50	150		34	200
	54	200		45	300
	56	250		55	500
82.5	38	100	97	34	235
	46	150		47	376
	50	200		52	458
	54	250		57	650
	56	300		61	830

Solubility of α -TNT in 100 g solvent^[88]:

T (°C)	H ₂ O	CCl ₄	Benzene	Toluene	Acetone	95% EtOH	CHCl ₃	Et ₂ O
0	0.0100	0.20	13	28	57	0.65	6	1.73
5	0.0105	0.25	24	32	66	0.75	8.5	2.08
10	0.0110	0.40	36	38	78	0.85	11	2.45
15	0.0120	0.50	50	45	92	1.07	15	2.85
20	0.0130	0.65	67	55	109	1.23	19	3.29
25	0.0150	0.82	88	67	132	1.48	25	3.80
30	0.0175	1.01	113	84	156	1.80	32.5	4.56
35	0.0225	1.32	144	104	187	2.27	45	—
40	0.0285	1.75	180	130	228	2.92	66	—
45	0.0360	2.37	225	163	279	3.70	101	—
50	0.0475	3.23	284	208	346	4.61	150	—
55	0.0570	4.55	361	272	449	6.08	218	—
60	0.0675	6.90	478	367	600	8.30	302	—
65	0.0775	11.40	665	525	843	11.40	442	—
70	0.0875	17.35	1,024	826	1,350	15.15	—	—

75	0.0975	24.35	2,028	1,685	2,678	19.50	–	–
80	0.1075	–	–	–	–	–	–	–
85	0.1175	–	–	–	–	–	–	–
90	0.1275	–	–	–	–	–	–	–
95	0.1375	–	–	–	–	–	–	–
100	0.1475	–	–	–	–	–	–	–

Values from^[27]:

Solvent	Solubility in g per 100 g solvent at °C							
	0	20	25	30	40	50	60	75
Ethanol (95%)	0.65	1.23	1.48	1.80	–	4.61	–	19.5
Ether	1.73	3.29	3.80	4.56	–	–	–	–
Acetone	57	109	132	156	–	346	–	–
CCl ₄	0.20	0.65	0.82	1.01	–	3.23	–	24.35
CHCl ₃	6	19	25	32.5	–	150	–	–
Ethylene chloride	–	18.7	22	29	–	97	–	–
Benzene	13	67	88	113	–	284	–	–
Toluene	28	55	67	84	–	208	–	–
CS ₂	0.14	0.48	0.63	0.85	–	–	–	–
Methyl acetate	–	72.1	80	99	–	260	–	–
Triacetin	–	–	37.7	–	–	–	–	–
Butyl carbitol acetate	–	24	–	–	–	–	–	–
Sulfuric acid	–	4	–	–	–	–	–	–
<i>N,N</i> -DMF	90	119 @ 150 °C	142	–	–	–	–	–
DMSO	–	–	128	–	–	–	–	–
1-Methyl-2-pyrrolidinone	–	–	118	–	–	–	–	–
Pyridine	–	137	–	–	–	–	–	–
Chlorobenzene	–	33.9	–	–	–	–	–	–

1,2-Dichloroethane	–	18.7	–	–	–	–	–	–
Et ₂ O	–	3.29	–	–	–	–	–	–
Trichloroethylene	–	3.04	–	–	–	–	–	–
MeOH	–	–	–	–	9.5	–	31.6	–

Solubility of TNT in binary solvent mixtures at 25 °C (g/100 g solvent after 5 min stirring)^[160]:

Solvent	TNT
DMSO	128
NMP	118
NMP 79.2% DMSO 20.8%	120
DMF	142
DMF 71.7% DMSO 28.3%	142

Solubility of TNT in DMF (g/100 g solvent) after 5 min stirring^[160]:

Explosive	0 °C	15 °C	25 °C
TNT	90	119	142

Solubility of TNT isomers (g) in 100 g alcohol^[162]:

T (°C)	Trinitrotoluene isomers		
	α - (2,4,6-)	γ - (2,4,5-)	β - (2,3,4-)
25	1.5	1.4	1.9
30	1.8	1.7	2.4
35	2.3	2.1	2.9
40	2.9	2.7	3.5
45	3.7	3.4	4.5
50	1.6	4.2	5.4
55	6.1	5.9	6.9
60	8.3	7.3	8.5
65	11.4	8.5	11.0
70	15.5	12.7	14.7

Solubility of TNT isomers (g) in 100 g of benzene and alcohol mixtures at 25 °C^[162]:

Benzene:alcohol ratio	1:1	1:2	1:3	1:9
2,4,6-TNT	20.4	8.7	5.3	2.5
2,4,5-TNT	12.2	6.6	4.7	2.3
2,3,4-TNT	9.5	6.4	4.7	2.9

Solubility of isomers of TNT (g) in 100 g toluene at 35 °C^[162]:

TNT isomer	2,4,6-TNT	2,4,5-TNT	2,3,4-TNT
Solubility	67.0	23.2	13.7

Solubility of isomers of TNT in various solvents^[162]:

TNT isomer	Solvent	T of soln. (°C)	Solubility (%)
1,3,8-	Dichloroethane	19	0.60
1,2,5-	Dichloroethane	19	3.72
1,3,8-	65% HNO ₃	19	0.07
1,2,5-	65% HNO ₃	19	0.25
1,2,5-	Chloroform	19	2.01
1,3,8-	Acetone	19	2.99
1,2,5-	Acetone	19	25.42
1,3,8-	95% Alcohol	19	0.02
1,2,5-	95% Alcohol	19	0.43
1,4,5-	Gasoline	55	0.07
1,2,5-	Gasoline	65	0.06
1,3,5-	Acetic acid	80	0.73
1,4,5-	Acetic acid	Boiling point	Insoluble
1,2,5-	Carbon disulfide	Boiling point	Insoluble
1,3,8-	Carbon disulfide	Boiling point	Insoluble
1,3,8-	Water	Boiling point	Insoluble
1,2,5-	Water	Boiling point	0.04

low solubility in H₂O^[163], 0.02 parts dissolve in 100 parts H₂O @ 15 °C^[163], 0.15 parts dissolve in 100 parts H₂O @ 100 °C^[163], best solvents for TNT are pyridine, acetone, benzene, toluene and CHCl₃^[163], poorly soluble in CS₂ and Et₂O^[163]

% solubility of α -TNT in Sulfuric acid of various % strengths^[163]:

T (°C)	% Solubility of TNT in sulfuric acid of different % strengths						
	70	75	80	85	90	95	100
0	–	0.30	0.40	0.6	2.0	3.5	13.0
10	–	0.30	0.45	0.7	2.2	4.0	13.5
20	–	0.30	0.50	0.8	2.5	4.8	15.0
25	–	0.32	0.55	0.9	2.6	5.2	15.5
30	–	0.35	0.60	1.0	2.7	6.0	16.5
40	0.2	0.40	0.65	1.3	3.0	7.0	18.0
50	0.2	0.45	0.70	1.7	3.5	8.5	21.0
60	0.22	0.50	1.00	2.3	5.2	11.0	24.0
70	0.35	0.70	1.60	3.3	7.0	13.5	29.0
80	0.60	1.30	2.40	4.8	10.0	18.0	36.5

very Soluble in nitric acid, even in dil. nitric acid^[163]:

% Strength HNO ₃	T (°C)	Solubility (g) of α -TNT in 100 g HNO ₃
78.2	48	100
	53	150
	56	200
	59	250
	61	300
80.4	44	100
	50	150
	54	250
	56	300
82.5	38	100
	46	150
	50	200
	54	250
	56	300

	<p>Data from^[25]:</p> <table><tr><th rowspan="2">Solvent</th><th colspan="3">g TNT dissolved/100 g solvent</th></tr><tr><th>20 °C</th><th>40 °C</th><th>60 °C</th></tr><tr><td>Acetone</td><td>109.0</td><td>228.0</td><td>600.0</td></tr><tr><td>Benzene</td><td>67.0</td><td>180.0</td><td>478.0</td></tr><tr><td>Butyl carbinol acetate</td><td>24.0</td><td>–</td><td>–</td></tr><tr><td>Carbon disulfide</td><td>0.48</td><td>1.53</td><td>–</td></tr><tr><td>Carbon tetrachloride</td><td>0.65</td><td>1.75</td><td>6.90</td></tr><tr><td>Chlorobenzene</td><td>33.9</td><td>–</td><td>–</td></tr><tr><td>Chloroform</td><td>19.0</td><td>66.0</td><td>302</td></tr><tr><td>Diethyl ether</td><td>3.29</td><td>–</td><td>–</td></tr><tr><td>Ethanol (95%)</td><td>1.23</td><td>2.92</td><td>8.30</td></tr><tr><td>Ethylene chloride</td><td>18.7</td><td>–</td><td>–</td></tr><tr><td>Hexane</td><td>0.16</td><td>–</td><td>–</td></tr><tr><td>Methyl acetate</td><td>72.1</td><td>–</td><td>–</td></tr><tr><td>Toluene</td><td>55.0</td><td>130.0</td><td>367.0</td></tr><tr><td>Trichloroethylene</td><td>3.04</td><td>–</td><td>–</td></tr><tr><td>Water</td><td>0.0130</td><td>0.0285</td><td>0.0675</td></tr></table>	Solvent	g TNT dissolved/100 g solvent			20 °C	40 °C	60 °C	Acetone	109.0	228.0	600.0	Benzene	67.0	180.0	478.0	Butyl carbinol acetate	24.0	–	–	Carbon disulfide	0.48	1.53	–	Carbon tetrachloride	0.65	1.75	6.90	Chlorobenzene	33.9	–	–	Chloroform	19.0	66.0	302	Diethyl ether	3.29	–	–	Ethanol (95%)	1.23	2.92	8.30	Ethylene chloride	18.7	–	–	Hexane	0.16	–	–	Methyl acetate	72.1	–	–	Toluene	55.0	130.0	367.0	Trichloroethylene	3.04	–	–	Water	0.0130	0.0285	0.0675
Solvent	g TNT dissolved/100 g solvent																																																																			
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Acetone	109.0	228.0	600.0																																																																	
Benzene	67.0	180.0	478.0																																																																	
Butyl carbinol acetate	24.0	–	–																																																																	
Carbon disulfide	0.48	1.53	–																																																																	
Carbon tetrachloride	0.65	1.75	6.90																																																																	
Chlorobenzene	33.9	–	–																																																																	
Chloroform	19.0	66.0	302																																																																	
Diethyl ether	3.29	–	–																																																																	
Ethanol (95%)	1.23	2.92	8.30																																																																	
Ethylene chloride	18.7	–	–																																																																	
Hexane	0.16	–	–																																																																	
Methyl acetate	72.1	–	–																																																																	
Toluene	55.0	130.0	367.0																																																																	
Trichloroethylene	3.04	–	–																																																																	
Water	0.0130	0.0285	0.0675																																																																	
Viscosity	<p>13.90 mPa s (@ 358 K)^[83], 0.139 Poise @ 85 °C^[23, 27, 149], 0.095 Poise @ 100 °C^[23, 27]</p> <p>Data from^[25]:</p> <table><tr><th>T (°C)</th><th>Viscosity (cP)</th></tr><tr><td>85</td><td>12.0–13.7</td></tr><tr><td>90</td><td>10.6–11.8</td></tr><tr><td>95</td><td>9.4–10.2</td></tr><tr><td>100</td><td>8.6–9.0</td></tr></table>	T (°C)	Viscosity (cP)	85	12.0–13.7	90	10.6–11.8	95	9.4–10.2	100	8.6–9.0																																																									
T (°C)	Viscosity (cP)																																																																			
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95	9.4–10.2																																																																			
100	8.6–9.0																																																																			
Hygroscopicity	<p>0.03% @ 30 °C with 90% RH^[23], nonhygroscopic^[88, 142], 0.05% H₂O absorbed when exposed to air saturated with water @ RT^[88], all isomers (α-, β-, γ-, δ-, ζ-) are nonhygroscopic^[88], ~ 0.05% and therefore does not require storage in an airtight container^[163]</p>																																																																			

Photosensitivity

Photolysis of aqueous solns. of TNT results in the formation of pink water^[27], solid TNT decomposes on exposure to light^[27], mpt. decreases from 80.0 to 79.5 °C after 2 weeks sunlight irradiation (*Kast*)^[88], mpt. decreases from 80 to 74 °C after exposure to sunlight in the open for 3 months^[88], TNT irradiated in absence of air in vacuum showed no change in mpt.^[88, 93], TNT exposed to light forms a product insoluble in benzene and H₂O^[88], exposure to sunlight in open tubes = slow dec.^[93], all isomers (α -, β -, γ -, δ -, ζ -) are light sensitive and turn brown on exposure to sun^[88]

complex mixtures formed on photolysis of TNT in dilute aqueous solutions using medium pressure mercury lamp and pyrex filter to eliminate $\lambda < 280 \text{ nm}$ ^[138], rate of phototransformation of TNT is inversely proportional to pH^[138], rate enhancement of 10–100 fold observed for TNT photolysis in natural waters probably due to presence of humic acids^[138], exposure to sunlight or UV radiation causes progressive discoloration and dec. shown by increasing impact sensitivity^[149]

Effect of light on freezing point and sensitivity of 2,4,6-TNT^[162]:

Exposure time (h)	Freezing point (°C)	Shock sensitivity ($p = 10 \text{ kg}$, $h = 25 \text{ cm}$) of sample in % Explosions	Deflagration T (°C)
0	80.1	10	295–298
65	79.3	6	295–298
165	78.7	20	293–295
300	78.3	21	293–295
450	76.7	32	285–290
512	76.4	30	280–285

Sunlight causes TNT to darken and affects the freezing temperature, but less effect on the flash point^[163], photoisomerization of TNT proposed to occur on exposure to sunlight^[163]

Radiation sensitivity	Properties of a saturated aq. TNT solution and its photolysates after treatment in continuous flow system ^[80] :				
	UV exposure (h)	pH	Color/clarity of solution	GC results TNT (ppm)	TLC results (TNT/no. of conversion products)
	0	6.0	Colorless/clear	90	TNT/0
	1	–	Rusty/turbid	1	TNT/5
	3	–	Amber/slightly turbid	0	Trace of TNT/3
	4	–	Yellow/clear	0	0/1 ^f
	6.5	–	Straw/clear	0	0/1 ^f
	10	–	Straw/clear	0	0/1 ^f
	22.5	–	Colorless/clear	0	0/1 ^f
	25	–	Colorless/clear	0	0/0
	27	–	Colorless/clear	0	0/0
	29	3.3	Colorless/clear	0	0/0
	^f = fluorescent product (375 nm) ^[80]				
	Properties of a saturated aq. TNT soln. and its photolysates after UV treatment in the continuous flow system (24 h) ^[80] :				
	UV exposure (h)	pH	Appearance of soln.	GC results TNT (ppm)	TLC results/ no. of conversion products
	0	6.0	Colorless, clear	109.5	TNT
	2	3.2	Rusty, turbid	0	Trace TNT/3
	4	3.1	Amber, clear	0	0
	6	3.2	Straw, clear	0	0
	24	3.3	Colorless, clear	0	0

UV continuous flow treatment of TNT solutions with varied acetone concentrations (average concentration of TNT samples at exposure time = 0 h is 107.6 ppm)^[80]:

% Acetone	Exposure time (h)			
	0.5	2.5	~ 5	21.5
	TNT (ppm)			
0.01	25.8	0.14	0.02	0
0.02	38.0	0.16	0.20	0
0.05	25.9	0.09	0.42	0
0.10	15.1	0.50	0	0
0.20	15.0	0.15	0	0
0.25	7.5	0.02	0	0
0.50	7.8	0.03	0	0
1.00	6.6	0.10	0	0

Effect of peroxide concentration on TNT elimination with different UV exposure times in the continuous flow system (average concentration of TNT samples at exposure time = 0h is 95 ppm)^[80]:

% H ₂ O ₂	UV exposure time						
	10 min	15 min	1 h	2 h	3 h	4 h	5 h
	TNT concentration (ppm)						
2.0	52.9	—	10.2	8.0	5.4	3.5	—
1.5	—	56.6	7.3	2.1	0.6	0.5	0.4
1.0	—	35.5	6.2	3.5	0.8	0.1	0
0.5	60.4	—	6.4	1.8	—	0	0
0.05	35.1	—	0	0	0	—	0
0.02	—	33.0	0.18	0	—	0	0
0.01	—	28.0	0.30	0.1*	—	0	0

*sample taken at 2.5 h and not 2 h

No drop in chemical stability after exposure to γ -rays with intensity of 3×10^4 Roentgens/h administering doses of 0.5–20 megaroentgens with total exposure times of 15–660 h (cobalt-60 source)^[149]

Data obtained from explosives after exposure to gamma radiation^[165]:

Weight of sample (g)	5
Vol. of gas produced (mL/g) in following times (days)	
10	0.02
20	0.04
30	0.06
40	0.08
50	0.11
90	0.20
Total irradiation time (days)	90
Purity of sample by chemical analysis (%)	
Original material	—
Irradiated material	—
Melting points, corrected (°C)	
Original material	82.1
Irradiated material	80.9
IS (P.A. apparatus) (in)	
Original material	13
Irradiated material	12
IS (B.M. apparatus) (cm)*	
Original material	95
Irradiated material	95
Sand test, 200 g bomb, g of sand crushed when sample was ignited by black powder fuse only	
Original material	—
Irradiated material	—
Sand test, 200 g bomb, g of sand crushed when sample was initiated by 0.30 g LA	
Original material	48.9
Irradiated material	50.1, explosion 1 out of 10 trials

TNT irradiated at ambient *T* using 0.41 MeV ¹⁹⁸₇₉Au γ-rays; volumes of gas produced measured during and after irradiation, amount of gas evolved as function of gamma dose^[182]:

Gamma energy absorbed, 10 ⁷ R	Gas evolved (ml/g) @ STP
1	< 0.1
2	< 0.1
3	< 0.1
4	< 0.1
9	0.1

Effect of 60 MeV electron irradiation on explosives, ^a = sample tested at 100 cm with NOL apparatus^[182]:

Weight (mg)	Dose (R)	Dose rate (R/s)	Weight loss	Color change	Test	Results
8.0	1.14 × 10 ⁹	1.7 × 10 ⁶	None	Caramel	Impact ^a	Explosion

Data from^[186]:

Exposure rate (R/h)	Total dose (R)	Vacuum stability test	
		100 °C (cc/g/40 h)	120 °C (cc/g/40 h)
6.4 × 10 ⁵	Control	0.10	0.46
	1.0 × 10 ⁷	0.14	
	1.0 × 10 ⁸	1.16	
	1.0 × 10 ⁹	4.22	

DTA for irradiated explosives @ 20 °C/min^[186]:

Total dose (R)	Endotherms		Exotherms	
	First		First	
	Onset (°C)	Peak (°C)	Onset (°C)	Peak (°C)
0	77	81	290	324
1.0 × 10 ⁷	77	81	280	321
1.0 × 10 ⁸	70	77, 79	260	315
1.0 × 10 ⁹	20	71	245	290

TGA for irradiated explosives^[186]:

Total dose (R)	Heating rate (°C/min)	Weight (mg)	Start of dec (°C)	10% weight loss T (°C)	Total weight loss (%)
0	20	7.4	135	190	99 @ 250 °C
1.0×10^7	20	7.4	135	190	96 @ 255 °C
1.0×10^8	20	8.7	115	185	95 @ 255 °C
1.0×10^9	20	7.1	110	173	86 @ 235 °C
0	50	8.4	150	212	97 @ 275 °C
0	80	9.6	160	224	98 @ 300 °C

Effect of gamma radiation on the mpt. and color^[186]:

Total dose (R)	mpt. (°C)	Color
0	81.5	Light yellow
1.0×10^7	80.5	Yellow
1.0×10^8	78.5	Dark yellow
1.0×10^9		Brownish yellow

IS for irradiated explosives, 50% fire height in inches, Bruceton method (P.A. apparatus, 2 kg mass)^[186]:

Total Co ⁶⁰ gamma dose (R)	\bar{X} mean (in)	σ std. dev. (in)
0	25.5	7.48
1.0×10^7	26.5	8.41
1.0×10^8	—	—
1.0×10^9	30.11	5.55

Effect of gamma radiation on explosion T (5 s explosion T in °C) and activation energy (kcal/mol)^[186]:

Total dose (R)	5 s explosion T (°C)	Apparent activation energy (kcal/mol)
0	396	21.70
1.0×10^7	389	15.05
1.0×10^8	394	18.37
1.0×10^9	345	19.23

	Effect of gamma radiation on rates of detonation ^[186] :																									
	<table><tr><th>Total dose (R)</th><th>Density (g/cc)</th><th>Density after irradiation (g/cc)</th><th>Rate of detonation (m/s)</th><th>Detonation pressure (kbar)</th></tr><tr><td>0</td><td>1.60</td><td>–</td><td>6,875</td><td>189</td></tr><tr><td>1.0×10^7</td><td>1.60</td><td>1.60</td><td>6,875</td><td>189</td></tr><tr><td>1.0×10^8</td><td>1.59</td><td>1.55</td><td>6,850</td><td>182</td></tr><tr><td>1.0×10^9</td><td>1.57</td><td>1.45</td><td>6,395</td><td>143</td></tr></table>	Total dose (R)	Density (g/cc)	Density after irradiation (g/cc)	Rate of detonation (m/s)	Detonation pressure (kbar)	0	1.60	–	6,875	189	1.0×10^7	1.60	1.60	6,875	189	1.0×10^8	1.59	1.55	6,850	182	1.0×10^9	1.57	1.45	6,395	143
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1.0×10^8	1.59	1.55	6,850	182																						
1.0×10^9	1.57	1.45	6,395	143																						
Compatibility	VST @ 110 °C, 20 h: RDX/TNT (60/40), @ 1.72 g cm ⁻³ , 99.0% TMD, vol. of gas = 0.13 cm ³ ^[115] , not adversely affected by moisture ^[142] , does not react with metals except in presence of dil. nitric acid ^[142] , reacts readily with alkaline solns. such as NH ₃ , NaOH, Na ₂ CO ₃ ^[142] , alkalies, alkoxides and ammonia react with TNT to form dangerous compounds ^[149] , solid TNT and KOH mixture bursts into flames on heating to 80 °C ^[149] , reacts with potassium methylate to form an explosive compound ^[149] , moisture has no effect on stability of TNT ^[149] , may cause slight corrosion of lead but has no corrosive effect on other metals, Shellac, acid-proof black paint or Bakelite ^[149] , unaffected by moisture ^[27] , unaffected by immersion in sea water ^[27] , reacts with EtOH @ 50 °C ^[27] , does not react with sulfuric acid @ RT but undergoes oxidation at elevated T ^[163] , strong mixed acid oxidizes TNT @ 115–130 °C ^[163] , reacts with alkaline solns. ^[163] , reacts with aqueous ammonia ^[163]																									
Wedge test [mm]	<p>2.06 (pressed TNT, LANL)^[85], cast TNT $\rho_0 = \sim 1.60$ g/cc, pressure = 137 kbar, run length (x_s) = 6.07 mm, $x_s^{-1} = 0.165$ mm^[170], cast TNT $\rho_0 = \sim 1.60$ g/cc, pressure = 75 kbar, run length (x_s) = 18.6 mm (chosen beyond plateau where steady state velocity is well established), $x_s^{-1} = 0.538$ mm^[170]</p> <p>Data from^[25]:</p> <table><tr><th>Density (g/cm³)</th><th>Distance, x^* and time t^* to detonation (mm and μs)</th><th>Pressure range (GPa)</th></tr><tr><td>1.1.62–1.634</td><td>$\log P = (1.40 \pm 0.03) - (0.32 \pm 0.03) \log x^*$ $\log P = (1.16 \pm 0.03) - (0.31 \pm 0.05) \log t^*$</td><td>91.7 < P < 17.1</td></tr></table> <p>where P = pressure in GPa</p> <p>$\rho = 1.654$ g cm⁻³, $a = 0.2109$ cm/μs, $b = 2.337$, $P_1 = 120$ kbar, slope = 3.125^[173]</p>	Density (g/cm ³)	Distance, x^* and time t^* to detonation (mm and μ s)	Pressure range (GPa)	1.1.62–1.634	$\log P = (1.40 \pm 0.03) - (0.32 \pm 0.03) \log x^*$ $\log P = (1.16 \pm 0.03) - (0.31 \pm 0.05) \log t^*$	91.7 < P < 17.1																			
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Minimum priming charge test [mg]	Data from ^[25] :		
	Density (g/cm ³)	W ₅₀ (mg of XTX 8003)	Comments
	1.59	394	Pressed @ 65 °C
	1.63	1,260	Pressed @ 65 °C
	375 (pressed TNT, LANL) ^[85]		
Bullet test [f/s]	4,700 (pressed TNT, LANL) ^[85]		
Steel bullet test	Comparison of values from gap tests and steel bullet tests ^[66]		
	Material	Velocity for 0.5 in diameter projectiles	
		Cylinders (ft/s)	Spheres (ft/s)
	Cast TNT	3,720 (est.)	6,924
	Pressed TNT ($\rho = 1.32 \text{ g cm}^{-3}$)	2,346 (est.)	2,913
Rifle bullet impact test	Rifle bullet impact sensitivity vs. temperature of confinement ^[23] :		
		Room temperature	105–110 °C
	<i>Standard iron bomb:</i>		
	No air space		
	Trials	10	10
	Explosions	1 very low order	7
	Air space		
	Trials	10	10
	Explosions	0	0
	<i>Tin or cardboard bombs:</i>		
	With or without air space		
	Trials	10	10
	Explosions	0	0
	Insensitive to rifle bullet impact if unconfined or confined in iron, tin or cardboard bombs ^[27] , insensitive to rifle bullet impact in tin or cardboard bombs or in iron bomb with an airspace @ 105–110 °C ^[27] , an iron bomb with no airspace showed explosion in 70% of trials ^[27] , 4% explosions, 0% partials, 0% burned, 6% unaffected in trials ^[23] , explodes in 2% trials ^[149] , 40% explosion, 0% partially exploded, 0% burned, 60% unaffected ^[165]		

Bullet impact test	Pressed TNT @ 1.58 g cm ⁻³ (96% TMD), bullet caliber = 7.82 mm, bullet velocity = 741 m/s, fracture scenario of metal case = ruptured in lids, reaction type = combustion ^[157]																																																																
Susan V-50 test [f/s]	425 (cast TNT, NWL/D) ^[85]																																																																
Susan LVR test [f/s]	1,220 (cast TNT, NWL/D) ^[85]																																																																
Plate dent test	<div>Data from^[23]:<table><tr><td>Plate dent test method</td><td>A</td><td>A</td><td>B</td></tr><tr><td>Condition</td><td>Cast</td><td>Pressed</td><td>Cast</td></tr><tr><td>Confined</td><td>Yes</td><td>Yes</td><td>No</td></tr><tr><td>Density, g/cc</td><td>1.61</td><td>1.50</td><td>1.61</td></tr><tr><td>Brisance, % TNT</td><td>100</td><td>100</td><td>100</td></tr></table></div> <div>Data from^[25]:<table><tr><th>Charge diameter (mm)</th><th>Density (g/cm³)</th><th>Dent depth (mm)</th><th>Charge height (mm)</th></tr><tr><td rowspan="4">12.7</td><td rowspan="4">1.63</td><td>1.57</td><td>12.7</td></tr><tr><td>1.70</td><td>16.9</td></tr><tr><td>1.93</td><td>84.59–508</td></tr><tr><td>2.90</td><td>203.0</td></tr><tr><td rowspan="13">25.4</td><td rowspan="13">1.631</td><td>1.73</td><td>12.7</td></tr><tr><td>2.90</td><td>25.4</td></tr><tr><td>3.20</td><td>31.7</td></tr><tr><td>4.04</td><td>42.4</td></tr><tr><td>4.19</td><td>50.8</td></tr><tr><td>4.27</td><td>63.5</td></tr><tr><td>4.14</td><td>72.6</td></tr><tr><td>4.19</td><td>84.6</td></tr><tr><td>4.09</td><td>101.6</td></tr><tr><td>4.11</td><td>127.0</td></tr><tr><td>4.14</td><td>169.4</td></tr><tr><td>4.06</td><td>254.0</td></tr><tr><td>4.09</td><td>508.0</td></tr></table></div>			Plate dent test method	A	A	B	Condition	Cast	Pressed	Cast	Confined	Yes	Yes	No	Density, g/cc	1.61	1.50	1.61	Brisance, % TNT	100	100	100	Charge diameter (mm)	Density (g/cm ³)	Dent depth (mm)	Charge height (mm)	12.7	1.63	1.57	12.7	1.70	16.9	1.93	84.59–508	2.90	203.0	25.4	1.631	1.73	12.7	2.90	25.4	3.20	31.7	4.04	42.4	4.19	50.8	4.27	63.5	4.14	72.6	4.19	84.6	4.09	101.6	4.11	127.0	4.14	169.4	4.06	254.0	4.09	508.0
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	0.205 mm crater depth ^[27] , 5.51 mm crater depth ^[98]																														
	Measured dent areas, dent volumes and dent depths ^[135] :																														
	<table><tr><td>Diameter (mm)</td><td>Area (mm²)</td><td>Volume (mm³)</td><td>Depth (mm)</td></tr><tr><td>74.98</td><td>6,439.29</td><td>36,844.76</td><td>13.37</td></tr><tr><td>74.79</td><td>6,801.88</td><td>38,652.68</td><td>13.43</td></tr><tr><td>74.8</td><td>6,518.61</td><td>37,364.75</td><td>12.95</td></tr><tr><td>50.42</td><td>2,832.78</td><td>10,238.27</td><td>8.46</td></tr><tr><td>50.62</td><td>2,825.25</td><td>10,239.24</td><td>8.70</td></tr><tr><td>50.42</td><td>2,826.32</td><td>10,239.98</td><td>8.39</td></tr></table>				Diameter (mm)	Area (mm ²)	Volume (mm ³)	Depth (mm)	74.98	6,439.29	36,844.76	13.37	74.79	6,801.88	38,652.68	13.43	74.8	6,518.61	37,364.75	12.95	50.42	2,832.78	10,238.27	8.46	50.62	2,825.25	10,239.24	8.70	50.42	2,826.32	10,239.98
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Plate push value [ft/s]	2,830 (@ 93% crystal ρ) ^[104] , 2,930 (@ 98% crystal ρ) ^[104]																														

Blast characteristics	Blast wave peak overpressure $P_{\max} = 5.1$ kPa (mean value) ^[103] , blast wave positive phase impulse $I^* = 0.73$ Pa s (mean value) ^[103]																											
Plastic properties	Properties of plastic material ≥ 150 °C ^[88] , 0–35 °C behaves as typical brittle material ^[88] , 35–40 °C (@ 45–47 °C for highly pure TNT) transition from brittle → plastic properties ^[88]																											
Dipole moment [D]	1.17 (calcd.) ^[111] , 1.37 (exptl.) ^[111]																											
Cylinder velocity	<div>Exptl. and calcd. velocities of cylinder, Cu cylinder, TNT @ 1.76 g cm^{-3}^[116]:</div> <table><tr><th rowspan="2">Source</th><th colspan="6">R–R⁰ (mm)</th></tr><tr><th>4</th><th>5</th><th>7</th><th>10</th><th>12</th><th>15</th></tr><tr><td>Exptl. value</td><td>1.17</td><td>1.23</td><td>1.29</td><td>1.35</td><td>1.38</td><td>1.41</td></tr><tr><td>Calcd. value</td><td>1.19</td><td>1.24</td><td>1.30</td><td>1.36</td><td>1.38</td><td>1.42</td></tr></table> <div>R_0 = initial value of outer radius of cylinder; R = current value of outer radius of cylinder</div>	Source	R–R ⁰ (mm)						4	5	7	10	12	15	Exptl. value	1.17	1.23	1.29	1.35	1.38	1.41	Calcd. value	1.19	1.24	1.30	1.36	1.38	1.42
Source	R–R ⁰ (mm)																											
	4	5	7	10	12	15																						
Exptl. value	1.17	1.23	1.29	1.35	1.38	1.41																						
Calcd. value	1.19	1.24	1.30	1.36	1.38	1.42																						
LAVA	Vol. of gas released during 40 h thermostating of 5 g TNT: $0.1 \text{ cm}^3/\text{g}$ @ 100 °C ^[123] , $0.4 \text{ cm}^3/\text{g}$ @ 120 °C ^[123] , $0.7 \text{ cm}^3/\text{g}$ @ 150 °C ^[123]																											
Bourdon manometer	0.03 mL/g @ 120 °C , 48 h ^[124]																											
Sled test	<div>Values from^[124]:</div> <table><tr><th>$\rho \text{ (g cm}^{-3}\text{)}$</th><th>Height (m)</th><th>Overpressure (kPa)</th><th>Strike area (mm²)</th><th>Reaction grade</th><th>Exptl. phenomena</th></tr><tr><td>1.64</td><td>4.3</td><td>0</td><td>29</td><td>0</td><td>No reaction</td></tr><tr><td>1.64</td><td>6.1</td><td>0</td><td>32</td><td>2.2</td><td>Obvious burnt marks on target and charge; fire and smoke</td></tr></table>	$\rho \text{ (g cm}^{-3}\text{)}$	Height (m)	Overpressure (kPa)	Strike area (mm ²)	Reaction grade	Exptl. phenomena	1.64	4.3	0	29	0	No reaction	1.64	6.1	0	32	2.2	Obvious burnt marks on target and charge; fire and smoke									
$\rho \text{ (g cm}^{-3}\text{)}$	Height (m)	Overpressure (kPa)	Strike area (mm ²)	Reaction grade	Exptl. phenomena																							
1.64	4.3	0	29	0	No reaction																							
1.64	6.1	0	32	2.2	Obvious burnt marks on target and charge; fire and smoke																							
Adiabatic self-heating	<div>Values from^[125]:</div> <table><tr><th>Sample</th><th>T range (°C)</th><th>Depth of conversion as °C self-heating</th><th>$\log_{10}C_a$ (w/kg)</th><th>E_a (kcal/mol)</th></tr><tr><td>Pure TNT</td><td>145–196</td><td>0–51</td><td>20.60</td><td>43.0</td></tr><tr><td>Remelted TNT</td><td>150–160</td><td>51–61</td><td>15.46</td><td>31.3</td></tr><tr><td>Re-remelted TNT</td><td>126–144</td><td>61–79</td><td>13.51</td><td>27.2</td></tr></table>	Sample	T range (°C)	Depth of conversion as °C self-heating	$\log_{10}C_a$ (w/kg)	E_a (kcal/mol)	Pure TNT	145–196	0–51	20.60	43.0	Remelted TNT	150–160	51–61	15.46	31.3	Re-remelted TNT	126–144	61–79	13.51	27.2							
Sample	T range (°C)	Depth of conversion as °C self-heating	$\log_{10}C_a$ (w/kg)	E_a (kcal/mol)																								
Pure TNT	145–196	0–51	20.60	43.0																								
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Re-remelted TNT	126–144	61–79	13.51	27.2																								

Gurney energy [kJ/kg]	2,795 (@ 1.590 g cm ⁻³ , cylinder test, impulse X-ray apparatus, 300 mm long tube, 25 mm internal diameter, 2.5 mm wall thickness) ^[129]																	
Gurney velocity [m/s]	2,364 (@ 1.590 g cm ⁻³ , cylinder test, impulse X-ray apparatus, 300 mm long tube, 25 mm internal diameter, 2.5 mm wall thickness) ^[129]																	
Diffusion coefficient (air) [cm ² /s]	0.064 (est.) ^[138]																	
Diffusion coefficient (water) [cm ² /s]	6.71 × 10 ⁻⁶ (est.) ^[138]																	
Thermal diffusivity	Values from ^[27] : <table><tr><td>Thermal diffusivity (cm²/s × 10⁴) @ 25 °C</td><td>ρ (g/cc)</td></tr><tr><td>19.7</td><td>0.64</td></tr><tr><td>15.0</td><td>0.783</td></tr><tr><td>12.1</td><td>0.980</td></tr></table>			Thermal diffusivity (cm ² /s × 10 ⁴) @ 25 °C	ρ (g/cc)	19.7	0.64	15.0	0.783	12.1	0.980							
Thermal diffusivity (cm ² /s × 10 ⁴) @ 25 °C	ρ (g/cc)																	
19.7	0.64																	
15.0	0.783																	
12.1	0.980																	
Log K _{ow}	2.99 ^[138] , 1.86 ^[138] , 1.84 ^[138] , 1.86–2.00 @ 25 °C ^[144] , 1.6 ^[152] , K _{ow} = 100 ^[175] , 2.0 ^[175]																	
Log K _{oc}	2.72 ^[138, 175] , K _{oc} = 524 ^[175]																	
Shock sensitivity	Sample weight = 36.4 mg, taper diameter = 0.153 in (initial), taper diameter = 0.165 in (final) taper angle = 3.9° (exploding foil slapper technique, 2 mil mylar disk driven by Al plasma; constant stunning voltage of 12 kV; taper angle = angle the inclined face of taper makes with the vertical) ^[140] , Sample weight = 36.8 mg, taper diameter = 0.153 in (initial), taper diameter = 0.167 in (final) taper angle = 4.4° (exploding foil slapper technique, 2 mil mylar disc driven by Al plasma; constant stunning voltage of 12 kV; taper angle = angle the inclined face of taper makes with the vertical) ^[140] , Sample weight = 37.1 mg, taper diameter = 0.154 in (initial), taper diameter = 0.167 in (final) taper angle = 4.1° (exploding foil slapper technique, 2 mil mylar disc driven by Al plasma; constant stunning voltage of 12 kV; taper angle = angle the inclined face of taper makes with the vertical) ^[140]																	
Refractive index	n ^D ₂₀ = 1.5430 (α-) ^[23, 27] , n ^D ₂₀ = 1.6742 (β-) ^[23, 27] , 1.717 (γ-) ^[27]																	
Booster sensitivity test	Values from ^[23] : <table><tr><td>Condition</td><td>Pressed</td><td>Cast</td></tr><tr><td>Tetryl, g</td><td>100</td><td>100</td></tr><tr><td>Wax, in for 50% detonation</td><td>1.68</td><td>0.82</td></tr><tr><td>Wax, g</td><td></td><td></td></tr><tr><td>Density, g/cc</td><td>1.55</td><td>1.60</td></tr></table>			Condition	Pressed	Cast	Tetryl, g	100	100	Wax, in for 50% detonation	1.68	0.82	Wax, g			Density, g/cc	1.55	1.60
Condition	Pressed	Cast																
Tetryl, g	100	100																
Wax, in for 50% detonation	1.68	0.82																
Wax, g																		
Density, g/cc	1.55	1.60																

	Pressed TNT, $\rho = 1.55 \text{ g cm}^{-3}$, 50% Gap = 1.68 in ^[165] , cast TNT, $\rho = 1.60 \text{ g cm}^{-3}$, 50% Gap = 0.82 in ^[165]																				
Coefficient of expansion	Values from ^[23] : <table><tr><td rowspan="2">Linear, %/°C</td><td>-40–60 °C</td><td>5.4×10^{-5}</td></tr><tr><td>-40–60 °C</td><td>6.7×10^{-5}</td></tr><tr><td rowspan="2">Volume, %/°C</td><td>27–80 °C</td><td>16×10^{-5}</td></tr><tr><td>16–70 °C</td><td>26.3×10^{-5}</td></tr></table> $5.0 \times 10^{-5} + 7.8 \times 10^{-8} T (1/^{\circ}\text{C}, @ T \text{ range } -40 < T < 60^{\circ}\text{C})^{[25]}$			Linear, %/°C	-40–60 °C	5.4×10^{-5}	-40–60 °C	6.7×10^{-5}	Volume, %/°C	27–80 °C	16×10^{-5}	16–70 °C	26.3×10^{-5}								
Linear, %/°C	-40–60 °C	5.4×10^{-5}																			
	-40–60 °C	6.7×10^{-5}																			
Volume, %/°C	27–80 °C	16×10^{-5}																			
	16–70 °C	26.3×10^{-5}																			
Hardness	1.4 (Moh's scale) ^[23, 27]																				
Compressive strength	13,800–14,000 lb/in ² , $\rho = 1.62 \text{ g/cc}^{[23]}$:																				
Armor plate impact test	Values from ^[23] : 60 mm mortar projectile: 50% inert velocity $\geq 1,100 \text{ ft/s}^{[23]}$ 500 lb general purpose bombs ^[23] : <table><tr><th>Plate thickness (in)</th><th>Trials</th><th>% inert</th></tr><tr><td>1</td><td>0</td><td></td></tr><tr><td>$1\frac{1}{4}$</td><td>0</td><td></td></tr><tr><td>$1\frac{1}{2}$</td><td>4</td><td>100</td></tr><tr><td>$1\frac{3}{4}$</td><td>4</td><td>50</td></tr></table>			Plate thickness (in)	Trials	% inert	1	0		$1\frac{1}{4}$	0		$1\frac{1}{2}$	4	100	$1\frac{3}{4}$	4	50			
Plate thickness (in)	Trials	% inert																			
1	0																				
$1\frac{1}{4}$	0																				
$1\frac{1}{2}$	4	100																			
$1\frac{3}{4}$	4	50																			
Bomb drop test	T7, 2,000 lb semi-armor-piercing bomb vs concrete: max safe drop = 5,000–6,000 ft ^[23] 500-lb general purpose bomb vs concrete ^[23] : <table><tr><td></td><td>No seal</td><td>Seal</td></tr><tr><td>Height, ft</td><td>4,000</td><td>4–5,000</td></tr><tr><td>Trials</td><td>26</td><td>20</td></tr><tr><td>Unaffected</td><td>24</td><td>20</td></tr><tr><td>Low order</td><td>2</td><td>0</td></tr><tr><td>High order</td><td>0</td><td>0</td></tr></table>				No seal	Seal	Height, ft	4,000	4–5,000	Trials	26	20	Unaffected	24	20	Low order	2	0	High order	0	0
	No seal	Seal																			
Height, ft	4,000	4–5,000																			
Trials	26	20																			
Unaffected	24	20																			
Low order	2	0																			
High order	0	0																			

	1,000-lb general purpose bomb vs concrete ^[23] :			
		No seal	Seal	
	Height, ft	5,000	5,000	
	Trials	21	26	
	Unaffected	18	22	
	Low order	0	0	
	High order	3	4	
100 kg drop test	10% firing: height = 6.5 ft, cast $\rho = 1.54 \text{ g cm}^{-3}$ ^[165]			
Fragmentation effects	Fragmentation effects of TNT, values from ^[27] :			
	Density (g/cc)	Pressed/cast	Average no. of fragments produced	Average velocity of fragments (m/s)
	1.54	Pressed	1,070	3,620
	1.58	Cast	1,850	3,570
Fragmentation test	Values from ^[23] :			
	90 mm HE, M71 projectile, Lot WC-91:			
	Density (g/cc)		1.60	
	Charge wt. (lb)		2.104	
	Total no. of fragments		703	
	3 in HE, M42A1 projectile, Lot KC-5:			
	Density (g/cc)		1.60	
	Charge wt. (lb)		0.848	
	Total no. of fragments		514	
Fragment velocity	Fragment velocity: ft/s ^[23] : 260 @ 9 ft, $\rho = 1.5 \text{ g/cc}$ ^[23] , 236 @ 25 ¹ / ₂ ft, $\rho = 1.5 \text{ g/cc}$ ^[23]			
Surface tension	Surface tension of liquid TNT ^[27] :			
	T (°C)		Surface tension (dynes/cm)	
	80		47.07	
	85		46.63	
	87.6		46.36	
	90		46.04	
	95		45.62	

Cylinder compression tests	3.5 mm compression (Cu cylinder) ^[27] , 16 mm compression (Pb cylinder) ^[27]
Fire fast cook-off test	Pressed TNT @ 1.58 g cm^{-3} (96% TMD), cook-off time = 360 s, cook-off temperature = 620 °C, fracture scenario of metal case = ruptured into block, cook-off reaction = deflagration ^[157]
Jet sensitivity test	Pressed TNT @ 1.58 g cm^{-3} (96% TMD), critical jet characteristics: X50 (steel plate thickness) = 97.2 mm, V_j (jet velocity) = 3.6 mm/ μs , d (jet diameter) = 1.4 mm, $V_j^2 d = 18.1 \text{ mm}^3/\mu\text{m}^2$ ^[157]
Small-Scale Cookoff Bomb test (SCB test)	Flake TNT, loose fill, heater voltage = 110, cookoff time = 11 min, cookoff reaction = detonation ^[158] , cast TNT, cookoff temperature ≥ 400 °C, cookoff time = 6.1 min, cookoff reaction = detonation ^[158]
Flash point [°C]	290 ^[163]
Shock sensitivity	4–8% explosions (@ 10 kg, h = 25 cm, 0.05 g sample, explodes on dropping a 2 kg mass from 100 cm height) ^[163]
Critical Lucite gap	Pressed TNT: 50% gap = 0.281 in, DBg = 5.52 (donor = RDX, 1 in long, 0.2 in diameter, pressed in steel @ 10 kpsi) ^[165] , cast TNT: 50% gap = 0.021 in, DBg = 16.7 (donor = RDX, 1 in long, 0.2 in diameter, pressed in steel @ 10 kpsi) ^[165]
Small-scale Lucite gap test	Cast TNT @ 1.5746 g cm^{-3} loading ρ , sensitivity = 16.5 DBg ^[165] , TNT @ 1.4078 g cm^{-3} loading ρ , loading pressure = 6.2 kpsi, sensitivity = 4.635 DBg ^[165] , TNT @ 1.5835 g cm^{-3} loading ρ , loading pressure = 19.0 kpsi, sensitivity = 6.114 DBg ^[165]
60 mm proj. against armor	1,100 ft/s ^[165]
T7 bomb max safe drop	5,000 ft ^[165]
Setback critical pressure	86.0 kpsi ^[165]
Combustion T [K]	Burn rate and equilibrium combustion temperature ^[166] : $T_e = 1,980 \text{ K}$ ^[166] , $m = 0.756 \text{ g cm}^{-2} \text{ s}^{-1}$ (100 atm.) ^[166]
Taliani test	100 °C bath temperature, 1.00 g Eastman TNT sample or 1.01 g military TNT sample, tube volume = 17.1 mL (Eastman TNT, sample no. 1), 17.3 mL (Eastman TNT, sample no. 2), 17.3 mL (military TNT, sample no. 3) or 17.5 mL (military TNT, sample no. 4), volume of gas evolved (cm^3) @ STP/g sample ^[167] :

	Time (h)	Volume of gas evolved (cm ³)			
		Eastman TNT (sample no.1)	Eastman TNT (sample no. 2)	Military TNT (sample no. 3)	Military TNT (sample no. 4)
	0	0.0	0.0	0.0	0.0
	¹ / ₆	0.1344	0.1335	0.0	0.0
	¹ / ₂	0.1344	0.1500	0.0	0.0
	1	0.1344	0.1670	0.0	0.0
	2	0.1344	0.1670	0.0	0.0
	5.5	0.1344	0.1670	0.0	0.0
	16	0.1680	0.1835	0.0167	0.0168
	17.5	0.2019	0.2170	0.0334	0.0336
	18.5	0.2019	0.2170	0.0501	0.0504
	19.5	0.2019	0.2170	0.0501	0.0504
	20.5	0.2019	0.2170	0.0501	0.0504
	22.5	0.2019	0.2170	0.0501	0.0504
	24	0.2019	0.2170	0.0501	0.0504
	40	0.2019	0.2170	0.0501	0.0504
	42	0.2019	0.2170	0.0501	0.0504
	48	0.2019	0.2170	0.0501	0.0504
	100 °C bath temperature, 1.00 g TNT (cycled) sample, tube volume = 21.3 mL, volume of gas evolved (cm ³) @ STP/g sample ^[167] :				
	Time (h)	Volume of gas evolved (cm ³)			
		TNT (cycled)		TNT (cycled)	
	¹ / ₂	0.0710		0.0304	
	16 ¹ / ₄	0.1055		0.0446	
	23	0.0913		0.0507	
	136	0.1602		0.0792	
Cylinder test	Data from ^[25] :				
	Density (g/cm ³)	Detonation velocity (mm/μs)	Cylinder wall velocity (mm/μs) at		
			R–R ₀ = 5 mm	R–R ₀ = 19 mm	
	1.630	6.940	1.18	1.40	

	TNT ^[37]	TNT ^[38]	TNT ^[39]	TNT ^[40]	TNT ^[5]	TNT ^[41]	TNT ^[41]	TNT ^[27, 163]	TNT ^[27, 163]
Chemical formula	C ₇ H ₅ N ₃ O ₆	C ₇ H ₅ N ₃ O ₆	C ₇ H ₅ N ₃ O ₆	C ₇ H ₅ N ₃ O ₆	C ₇ H ₅ N ₃ O ₆	C ₇ H ₅ N ₃ O ₆	C ₇ H ₅ N ₃ O ₆	C ₇ H ₅ N ₃ O ₆	C ₇ H ₅ N ₃ O ₆
Molecular weight [g mol ⁻¹]	227.13	227.13	227.13	227.13	227.13	227.13	227.13	227.13	227.13
Crystal system	Monoclinic	Monoclinic	Orthorhombic	Monoclinic	Orthorhombic	Monoclinic	Orthorhombic	Monoclinic	Orthorhombic
Space group	<i>P</i> 2 ₁	<i>C</i> 2/ <i>c</i> (no. 15)		<i>P</i> 2 ₁ / <i>c</i> (no. 14)		<i>P</i> 2 ₁ / <i>a</i>	<i>P</i> <i>c</i> <i>a</i> 2 ₁ (no. 29)	<i>P</i> 2 ₁ / <i>c</i> (no. 14)	<i>Pmca</i>
<i>a</i> [Å]	20.2	40.5	14.85	21.230(14)	40.0	14.9113(1)	14.910(2)	21.35 ± 0.05	20.07 ± 0.08
<i>b</i> [Å]	6.2	6.19	39.5	6.081(2)	14.89	6.0340(1)	6.031(2)	6.05 ± 0.03	6.09 ± 0.04
<i>c</i> [Å]	7.7	15.2	5.96	14.958(5)	6.09	20.8815(3)	19.680(4)	14.96 ± 0.05	15.03 ± 0.07
α [°]	90	90	90	90	90	90	90	90	90
β [°]	90.0*	90.52	90	110.12(2)	90	110.365(1)	90	111.15	90
γ [°]	90	90	90	90	90	90	90	90	90
<i>V</i> [Å ³]	964.348	3,810.41	3,495.99	1,813.23	3,627.2	1,761.37(4)	1,770.6(7)		
<i>Z</i>	4	16	16	8		8	8	8 (assumed)	8 (assumed)
ρ_{calc} [g cm ⁻³]	1.564	1.584	1.726	1.664		1.713	1.704	1.673 (based on <i>Z</i> = 8)	1.642 (based on <i>Z</i> = 8)
<i>T</i> [K]	295	295	295	295	295	100	123		
					Crystals obtained from soln. of TNT in benzene			Vacuum sublimation on surface maintained @ 78 °C	Dropping an acetone/TNT soln. into Et ₂ O or EtOH @ acetone/dry ice bath temperature

* Stated in the literature as monoclinic

Form-III is probably a mix of Form-I and Form-II^[41]. Twinning is so prevalent in TNT that large unit cells have been erroneously postulated in the past^[41]. Orthorhombic-TNT can remain stable for >12 months @ ambient temperature with transforming^[41]. According to ^[33], at least 7 morphological types of TNT have been identified^[33].

Crystal type obtained: sublimation onto condensing surface @ 78 °C forms monoclinic crystals^[33]; freezing melts close to mpt. forms monoclinic crystals^[33], recrystallization from solvents @ RT mainly forms monoclinic crystals^[33], strongly super-cooled melts form mainly monoclinic crystals^[33]; recrystallization from organic solvents @ low T forms orthorhombic crystals^[33].

	TNT ^[5]	TNT ^[25]	TNT ^[5]
Chemical formula	C ₇ H ₅ N ₃ O ₆	C ₇ H ₅ N ₃ O ₆	C ₇ H ₅ N ₃ O ₆
Molecular weight [g mol ⁻¹]	227.13	227.13	227.13
Crystal system	Orthorhombic	Orthorhombic*	Monoclinic
Space group	<i>P</i> 2 ₁ <i>ca</i>		<i>P</i> 2 ₁ / <i>b</i>
<i>a</i> [Å]	20.041(20)	15.007	21.407(20)
<i>b</i> [Å]	15.013(8)	20.029	15.019(8)
<i>c</i> [Å]	6.0836(5)	6.098	56.0932(5)
α [°]	90	90	90
β [°]	90	90	90
γ [°]	90	90	111.00(20)
<i>V</i> [Å ³]	1,830.45		1,828.86
<i>Z</i>	8		8
ρ_{calc} [g cm ⁻³]	1.647	1.646	1.648
<i>T</i> [K]	295		295
	Crystals obtained from gas-phase		Crystals grown from dichloromethane

* Controversial: may be a disordered monoclinic polymorph^[25]

TNT exists in two main crystalline forms^[35]:

- Monoclinic form which is stable @ RT up to the mpt. of 81 °C (usually shows extensive twinning)
- Orthorhombic form which is metastable @ RT, but which undergoes a solid-solid phase transition >70 °C before melting @ 81 °C. An orthorhombic → monoclinic phase transition can be observed in crystals^[35]

In each polymorph there are two types of TNT molecule present: four type-A molecules and four type-B molecules. Both types have three different types of –NO₂ groups^[35].

	TNT ^[35]	TNT ^[35]	TNT ^[35]	TNT ^[35]	TNT ^[35]
	Monoclinic forms		Orthorhombic forms		
Chemical formula	C ₇ H ₅ N ₃ O ₆	C ₇ H ₅ N ₃ O ₆	C ₇ H ₅ N ₃ O ₆	C ₇ H ₅ N ₃ O ₆	C ₇ H ₅ N ₃ O ₆
Molecular weight [g mol ⁻¹]	227.13	227.13	227.13	227.13	227.13
Crystal system	Monoclinic	Monoclinic	Orthorhombic	Orthorhombic	Orthorhombic
Space group	P 2 ₁ / c (no. 14)	P 2 ₁ / c (no. 14)	Pb21a	P2 ₁ ca	
a [Å]	21.275	21.407	15.005	20.041	40.0
b [Å]	6.093	15.019	20.024	15.013	14.89
c [Å]	15.025	6.0932	6.107	6.0836	6.09
α [°]	90	90	90	90	90
β [°]	110.23	111.00	90	90	90
γ [°]	90	90	90	90	90
V [Å ³]					
Z	8	8	8	8	
ρ _{calc} [g cm ⁻³]					
T [K]					
Authors	Duke in Gallagher <i>et al.</i>	Golovina <i>et al.</i>	Duke in Gallagher <i>et al.</i>	Golovina <i>et al.</i>	Golovina <i>et al.</i>

Comparison of some of the crystallographic constants reported for TNT, data from^[179]:

	<i>Carper et al. (1982)</i>	<i>Golovina et al. (1994)</i>	<i>Duke (1981)^b</i>
Orthorhombic form			
<i>a</i> (Å)	14.991(2)	20.041(20)	15.005(2)
<i>b</i> (Å)	6.077(1)	15.013(8)	20.024(4)
<i>c</i> (Å)	20.017(2)	6.084(5)	6.107(3)
Space group	<i>Pca</i> 2 ₁	<i>P</i> 2 ₁ <i>ab</i>	<i>Pb</i> 2 ₁ <i>a</i>
R-factor	0.057	0.055	0.043
Monoclinic form			
<i>a</i> (Å)		21.407(20)	21.275(2)
<i>b</i> (Å)		15.019(8)	6.093(3)
<i>c</i> (Å)		6.0932(5)	15.025(1)
Monoclinic angle (°)		(γ) 111.00(2)	(β) 110.14
Space group		<i>P</i> 2 ₁ / <i>b</i>	<i>P</i> 2 ₁ / <i>c</i>
R-factor		0.061	0.049

TNT crystallizes in two basic polymorphic forms: Orthorhombic *Pb*2₁*a* (*a* = 15.005 Å, *b* = 20.024 Å, *c* = 6.107 Å) and monoclinic *P*2₁/*c* (*a* = 21.275 Å, *b* = 6.093 Å, *c* = 15.025 Å, β = 110.23°)^[177] and depending on the crystallization conditions, TNT may form crystals of the separate phases or form complex mixed phase crystals^[177], crystals obtained from solvents are either monoclinic, orthorhombic or twinned monoclinic depending on the solvent which is used^[177]

Orthorhombic and monoclinic TNT have been isolated^[25]; monoclinic obtained from annealing cast TNT^[25], crystallization from most common organic solvents results in complex mixed-phases and (usually) disordered twinned crystals^[25], monocrystals obtained from cyclohexanone^[25], orthorhombic polymorph is controversial and may only be a disordered version of the monoclinic polymorph^[25]: Monoclinic, *a* = 21.275 Å, *b* = 6.093 Å, *c* = 15.025 Å, β = 110.14°, *Z* = 8^[25], Orthorhombic, *a* = 15.007 Å, *b* = 20.029 Å, *c* = 6.098 Å^[25]

The influence of crystallization solvent on the morphology of TNT crystals^[177]:

Solvent	Habit	Color	Polymorph	Twinned
Ethylacetate	Lozenge	Faint yellow	Monoclinic	Yes/no
Methanol	Needles, rods, plates	Dark amber	Monoclinic	Yes
Toluene	Plates	Yellow	Monoclinic	Yes
Acetone	Needles, rods, plates	Amber	Monoclinic	Yes
Ethanol	Needles, rods, plates	Amber	Orthorhombic	–
Cyclohexanol	Needles, rods, plates	Amber	Orthorhombic	–

Crystal types obtained (hot solution of TNT in methanol is introduced into a different medium)^[88]:

TNT/MeOH soln. is poured into	Average dimensions of crystals formed (μ)	Limits of dimensions of crystals formed (μ)	Ratio of axes length/width
Solid CO ₂	29	3.5430	9.6
H ₂ O	25	6.60	3.0

Crystallization data for TNT^[156]:

Solvent	Habit	Size (mm ³)	Color	Polymorph	Twinned
Ethylacetate	Coffin-like	47 × 10 × 3	Faint yellow	Monoclinic	Yes/no
Methanol	Needles, rods, plates	5 × 4 × 1	Dark amber	Monoclinic	Yes
Toluene	Plates	10 × 10 × 2	Yellow	Monoclinic	Yes
Acetone	Needles, rods, plates	5 × 4 × 1	Amber	Monoclinic	Yes
Ethanol	Needles, rods, plates	2 × 1 × 0.25	Amber	Monoclinic and orthorhombic	Yes
Cyclohexanol	Needles	2 × 0.5 × 0.5	Amber	Orthorhombic	Yes

Failure diameters of lead and booster explosives^[165]:

Explosive	Bare, in	Confinement, in		
		Fabric detonating cord	Lucite	Heavy brass or steel
TNT (granular)	0.50–0.70	<0.63	0.50	<0.10
TNT (25 μ)			<0.10	—

The charge preparation method affects the infinite-diameter detonation velocity and failure diameter of unconfined cylindrical charges as follows^[25]:

Method of charge preparation	Charge density (g/cm ³)	Detonation velocity at infinite "D" (mm/μs)	Critical diameter (mm)
Vacuum melting	–	–	–
Creaming and casting	1.615	6.942 ± 0.028	14.6 ± 2.0
Vacuum melting and casting	1.620	6.999 ± 0.011	14.5 ± 0.5
Pressing	1.620	7.045 ± 0.170	2.6 ± 0.6
Liquid	1.443	6.574 ± 0.001	62.6 ± 2.6

Effect of charge radius: detonation velocity varies with charge radius and preparation procedure as follows^[25]:

Method of charge preparation	Density (g/cm ³)	Effect of charge radius on detonation velocity (mm/μs)
Creaming and casting	1.615	$D(R) = 6.942 [(1 - 5.67 \times 10^{-2}/R) - 4.2 \times 10^{-1}/R (R - 7.41)]$
Vacuum melting and casting	1.620	$D(R) = 6.999 [(1 - 1.3 \times 10^{-2}/R) - 6.2 \times 10^{-1}/R (R - 5.5)]$
Pressing	1.620	$D(R) = 7.045 [(1 - 6.1 \times 10^{-2}/R) - 3.5 \times 10^{-2}/R (R - 0.57)]$
Liquid	1.443	$D(R) = 6.574 (1 - 0.291/R)$

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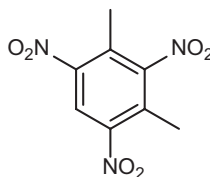
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Trinitroxylene

Name [German, acronym]: Trinitroxylene, 1,3-dimethyl-2,4,6-trinitrobenzene, 2,4,6-trinitro-*m*-xylene, xylyl, 2,4,6-trinitroxylene [trinitroxytol, TNX[†]]

Main (potential) use: Component in bursting charges, component of AN explosives^[19], was used in hand grenades, mines and shells^[19], component of dynamites^[13], additive to fusible explosive compositions^[14]

Structural formula:



[†] 2,4,6-Trinitro-*m*-xylene is the main component of commercial TNX, only insignificant quantities of the 4,5,6-TNX isomer are present in addition to 2,4,5-TNX.

	TNX
Formula	C ₈ H ₇ N ₃ O ₆
Molecular Mass [g mol ⁻¹]	241.16
Appearance at RT	large colorless needles if recryst. from benzene ^[13] , white crystals ^[14] , fine white or slightly yellowish crystalline solid (technical) ^[19]
IS [J]	10.46 ^[3] , 9.90 (first reaction) ^[5, 16] , 10.46 (sound) ^[5, 16] , more sensitive than PA (i.e. if PA assigned sensitivity = 100, then TNX = 120) ^[14] , 75.0 cm (2.5 kg mass, AFATL) ^[17]
ESD [J]	11.10 ^[3] , 11.1 ^[4, 21]
N [%]	17.42
Ω(CO ₂) [%]	-89,57
T _{m.p.} [°C]	180.2 ^[1] , 187 ^[9] , 182.3 ^[13] , 120–125 (partial melting, commercial TNX) ^[14] , 160–177 (complete melting, commercial TNX) ^[14] , 160–162 (solidification, commercial TNX) ^[14] , 170 (grade I TNX) ^[14] , 160–162 (grade II TNX) ^[14] , 182 (chemically pure) ^[14] , 182 (2,4,6-TNX) ^[14] , 90 (2,4,5-TNX) ^[14] , 125 (4,5,6-TNX) ^[14] , 170–176 (purified technical product, freezing point) ^[19] , 170–180 (melts without dec.) ^[19]
T _{dec.} [°C]	521 K (DTA @ 5 °C/min) ^[5, 16] , 351 (exotherm peak max, DSC @ 20 °C/min) ^[9]
ρ [g cm ⁻³]	1.623 ^[2] , 1.69 ^[8] , sp. gr. = 1.65 ^[19] , gravimetric density = 0.6 ^[19]

Heat of formation	−102.6 kJ/mol ^[6] , −425.6 kJ/kg (enthalpy of form.) ^[8] , 18.3 kcal/mol (ΔH_f) ^[14]	
	Calcd. (EXPLO5 6.04)	Exptl.
− $\Delta_{\text{ex}}U^\circ$ [kJ kg ^{−1}]	4,050	3,533 [H ₂ O (l)] ^[6, 8] 3,391 [H ₂ O (g)] ^[8]
T_{ex} [K]	2,876	
$p_{\text{C-J}}$ [kbar]	164	
VoD [m s ^{−1}]	6,527 (@ 1.623 g cm ^{−3} , $\Delta_f H = -102.6$ kJ mol ^{−1})	6,600 (@ 1.51 g cm ^{−3} , average lit. value) ^[10, 14] 6,613 (calcd., based on sand expts.) ^[10]
V_0 [L kg ^{−1}]	649	843 ^[7, 8]

Trauzl test [cm ³ , % TNT]	93% TNT ^[10] , 270 mL ^[14, 19, 20]												
Sand test [g]	84% TNT ^[10] , 34.5 g sand crushed (1,700 g bomb, 0.4 g TNX) ^[10]												
Initiation efficiency	Amount (g) of primary explosive necessary to cause detonation of TNX ^[15] : 0.25 g silver azide ^[15] , 0.40 g cuprous azide ^[15] , 0.50 g mercurous azide ^[15] , 0.30 g silver fulminate ^[15] , 0.35 g cadmium fulminate ^[15] , 0.43 g copper fulminate ^[15] , 0.40 g mercury fulminate ^[15]												
5 s explosion <i>T</i> [°C] 5 s ignition <i>T</i> [°C] Initiation <i>T</i> [°C] Detonation point [°C]	315–330 ^[11] 315–330 ^[11] 330 ^[14] ~330 °C ^[19]												
Thermal stability	No. of moles gas produced per mole TNX/no. h ^[9] : @ 120 °C: 0/22, 0/72 ^[9] , @ 220 °C: 1.01/22, 1.660/72 ^[9] , @ 320 °C: 2.13/22, 2.22/72 ^[9]												
Sublimation	Can be purified by sublimation @ 150–170 °C ^[14]												
Solubility [g/mL]	<p>Slightly soluble in conc. H₂SO₄^[14], 0.024 g dissolves in 100 mL 95% EtOH @ 8 °C^[14]</p> <p>Solubility (g) of TNX in 100 mL solvent^[14]:</p> <table><tr><td>Solvent</td><td>@ RT</td><td>@ bpt. of solvent</td></tr><tr><td>Benzene</td><td>0.5</td><td>7.5</td></tr><tr><td>Toluene</td><td>0.5</td><td>20.5</td></tr><tr><td>Alcohol</td><td>0.05</td><td>0.55</td></tr></table>	Solvent	@ RT	@ bpt. of solvent	Benzene	0.5	7.5	Toluene	0.5	20.5	Alcohol	0.05	0.55
Solvent	@ RT	@ bpt. of solvent											
Benzene	0.5	7.5											
Toluene	0.5	20.5											
Alcohol	0.05	0.55											

	Solubility (g) of TNX in 100 mL benzene/alcohol mixed solvent ^[14] :			
	Composition of the solvent (parts per volume)		Solubility (g)	
	Benzene	Alcohol	@ 8 °C	@ 20 °C
	1	0.5	–	0.71
	1	1	0.32	0.45
	1	1.5	0.24	0.29
	1	2	–	0.2
	Virtually insoluble in water ^[19] , poorly soluble in EtOH and EtOH/benzene mixtures ^[19] , good solubility in benzene and acetone ^[19]			
	Volumetric ratio of solubility of xylyl at various temperatures ^[19] :			
	Alcohol	Benzene	T (°C)	
			20	80
		0.5	1	0.71
		1.0	1	0.15
		1.5	1	0.29
		2.0	1	0.2
Compatibility	Does not react with metal ^[19] , reacts with alcoholic bases ^[19] , does not react with gaseous NH ₃ ^[19] , low T and moisture facilitate reaction with NH ₃ ^[19]			
Dipole moment [D]	1.27 (calcd.) ^[17]			
Closed vessel test	Gas pressure (exptl.) by exploding samples in small bombs, pressure measured by piston and obturator ^[12] : loading $\rho = 0.20 \text{ g cm}^{-3}$, pressure = 1,635 kg/cm ² ^[12] , loading $\rho = 0.25 \text{ g cm}^{-3}$, pressure = 2,340 kg/cm ² ^[12] , loading $\rho = 0.30 \text{ g cm}^{-3}$, pressure = 2,980 kg/cm ² ^[12]			

	TNX^[2]
Chemical formula	C ₈ H ₇ N ₃ O ₆
Molecular weight [g mol ⁻¹]	241.16
Crystal system	Orthorhombic

Space group	<i>Pbcn</i>
<i>a</i> [Å]	5.749(2)
<i>b</i> [Å]	15.043(3)
<i>c</i> [Å]	11.415(2)
α [°]	90
β [°]	90
γ [°]	90
<i>V</i> [Å ³]	987.2(3)
<i>Z</i>	4
ρ_{calc} [g cm ⁻³]	1.623
<i>T</i> [K]	

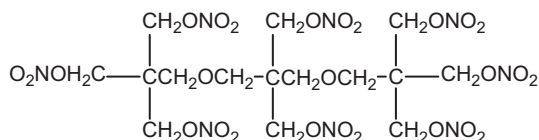
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Tripentaerythritol octanitrate

Name [German, acronym]: Tripentaerythritol octanitrate, pentaerythrit-3-ol octanitrate, tripentylerythritol [TPEON, TriPEON]
 Main (potential) use: High explosive, possible plasticizer for nitrocellulose^[1, 10], since it can be melted and poured it can be used for coating and sensitizer for AN^[5, 10]

Structural formula:



	TPEON
Formula	$\text{C}_{15}\text{H}_{24}\text{N}_8\text{O}_{26}$
Molecular mass [g mol ⁻¹]	732
Appearance at RT	White crystals ^[8] , irregularly-shaped agglomerates (crude product prepared from aqueous, acetone or alcohol soln.) ^[11] , clear-cut prism crystals obtained from hot CHCl_3 ^[11] , needles (recrystl. from hot EtOH) ^[12] , granular prism crystals (recryst. from CHCl_3) ^[12]
IS [J]	9 in (2 kg mass, 24 mg sample, P.A.) ^[1, 8] , 10 in (2 kg mass, 12 mg sample, P.A.) ^[8] , 20 cm (2 kg hammer) ^[6] , 23 cm (lower limit, 2 kg mass, P.A.) ^[10] , 40 cm (2 kg mass, detonation) ^[11] , 26 ± 0.02 cm (type 12A) ^[12] , 28 ± 0.10 cm (type 12B) ^[12]
FS [N]	Unaffected by steel shoe or fiber shoe (friction pendulum test) ^[1]
N [%]	15.31
$\Omega(\text{CO}_2)$ [%]	-34.97
T _{phase transition} [°C]	Four polymorphs identified using hot stage microscopy ^[9] , 4 crystalline morphologies ^[10] , crystal I is stable ^[10]
T _{m.p.} [°C]	82–84 ^[1, 3, 11] , 71–74 (crude TPEON) ^[3] , 82–83 ^[5] , four polymorphs identified with following mpts.: 83.3 (form I), 72.1 (form II), 74.6 (form III), 69.0 (form IV) ^[9] , 79–80 (clusters of needles by recrystallization from hot EtOH) ^[12] , 81–82 (granular prism crystals from CHCl_3) ^[12]

	mpt. (°C) of different crystal types of TPEON ^[10] :			
	I	II	III	IV
	83	76–77	68–70	64–65
	83.3	74.6	72.1	69.0
$T_{dec.}$ [°C]	215–250 (DSC @ 5 °C/min) ^[1]			
ρ [g cm ⁻³]	1.58 (crystal) ^[1] , 1.58 (abs.) ^[3] , 1.565 (loading ρ @ 60,000 psi) ^[3, 11] , 1.58 (crystal I) ^[10]			
Heat of formation	–1,705 kJ/kg ($\Delta_f H^\circ$, ICT thermochemical database) ^[7]			
Heat of combustion	2,632 cal/g (C ^V) ^[1, 3]			
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.	
$-\Delta_{ex}U^\circ$ [kJ kg ⁻¹]		1,400 ^[6] 6,306 J/g (calcd., ICT-code) ^[7] 1,085 kcal/kg ^[10]	1,058 cal/g ^[1, 3]	
T_{ex} [K]		3,900 (units not given) ^[6] 3,953 (calcd., ICT-code) ^[7]		
p_{C-J} [kbar]		12,000 kg/cm ² (specific pressure) ^[6] 133.3 MPa (calcd., ICT-code) ^[7]		
VoD [m s ⁻¹]		7,340 (@ 1.58 g cm ⁻³ (TMD), calcd., R-P method) ^[4] 8,340 (@ 1.7 g cm ⁻³) ^[6] 7,650 (@ 1.56 g cm ⁻³) ^[10]	7,650 (@ 1.56 g cm ⁻³ , 0.5 in charge diameter, pressed, no confinement) ^[1, 3] 7,710 ^[2]	
V_0 [L kg ⁻¹]		780 (specific gas volume, N_L /kg) ^[6]	762 cc/gm ^[1, 3]	

Trauzl test [cm ³ , % TNT]	515 (cf. TNT = 285) ^[6]																											
Sand test [g]	58.9 g sand crushed (cf. 48.0 g by TNT, 200 g sand bomb test) ^[3]																											
Initiation efficiency	0.30 g LA minimum detonating charge ^[1]																											
5 s explosion <i>T</i> [°C] Detonation <i>T</i> [°C]	225 ^[1, 3, 10] 215 ^[6]																											
Thermal induction periods for initiation [<i>T</i> (°C)/time (s)]	210/0 ^[3] , 215/9.3 ^[3] , 220/6.5 ^[3] , 230/4.1 ^[3] , 240/2.6 ^[3] , 250/2.0 ^[3]																											
100 °C heat test [% mass loss]	1.15 in first 48 h ^[1, 3] , 0.75 in second 48 h ^[1, 3] , no explosion in 100 h ^[1, 3]																											
Vacuum stability test [cm ³ /h]	2.45 cc/40 h @ 100 °C (pure) ^[1, 10] , 1.94 cc/40 h @ 120 °C (specially purified) ^[1, 10] , @ 100 °C: 6.24 mL gas evolved/40 h (5 g sample, crude TPEON) ^[3] , @ 100 °C: 2.45 mL gas evolved/40 h (5 g sample, pure TPEON) ^[3] , @ 120 °C: 1.94 mL gas evolved/40 h (5 g sample, specially purified TPEON) ^[3]																											
Solubility [g/mL]	<div>Solubility data from^[1]:</div> <table><tr><td>Solvent</td><td>Solubility</td></tr><tr><td>Water</td><td>Insoluble</td></tr><tr><td>Alcohol</td><td>Soluble</td></tr><tr><td>Chloroform</td><td>Soluble</td></tr><tr><td>Acetone, hot</td><td>Very soluble</td></tr><tr><td>Benzene, hot</td><td>Very soluble</td></tr></table> <div>Readily soluble in hot benzene and acetone^[5, 8], soluble in EtOH, CHCl₃^[5, 8], insoluble in H₂O^[5, 8], recryst. from CHCl₃ possible^[1], insoluble in water^[10, 11], soluble in EtOH, CHCl₃^[10], easily soluble in hot benzene and acetone^[10, 11], soluble in CHCl₃^[11], recryst. from EtOH or CHCl₃^[12]</div>	Solvent	Solubility	Water	Insoluble	Alcohol	Soluble	Chloroform	Soluble	Acetone, hot	Very soluble	Benzene, hot	Very soluble															
Solvent	Solubility																											
Water	Insoluble																											
Alcohol	Soluble																											
Chloroform	Soluble																											
Acetone, hot	Very soluble																											
Benzene, hot	Very soluble																											
Hygroscopicity	<div>Hygroscopicity, gain or loss in wt. %^[1]:</div> <table><tr><th rowspan="2">Time, h</th><th colspan="3">% RH @ 30 °C</th></tr><tr><th>40</th><th>70</th><th>90</th></tr><tr><td>24</td><td>−0.008</td><td>+0.01</td><td>+0.04</td></tr><tr><td>48</td><td>−0.02</td><td>−0.01</td><td>+0.02</td></tr><tr><td>144</td><td>−0.04</td><td>−0.03</td><td>−0.02</td></tr><tr><td>192</td><td>−0.04</td><td>−0.02</td><td>−</td></tr><tr><td>216</td><td>−0.004</td><td>−0.01</td><td>+0.03</td></tr></table>	Time, h	% RH @ 30 °C			40	70	90	24	−0.008	+0.01	+0.04	48	−0.02	−0.01	+0.02	144	−0.04	−0.03	−0.02	192	−0.04	−0.02	−	216	−0.004	−0.01	+0.03
Time, h	% RH @ 30 °C																											
	40	70	90																									
24	−0.008	+0.01	+0.04																									
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144	−0.04	−0.03	−0.02																									
192	−0.04	−0.02	−																									
216	−0.004	−0.01	+0.03																									

Specific impulse	240 lb-sec/lb (calcd.) ^[1]
Heat of fusion [cal/g]	18 (form I) ^[9] , 13 (form II) ^[9] , 13.1 (form III) ^[9] , ~ 10.5 (form IV) ^[9]

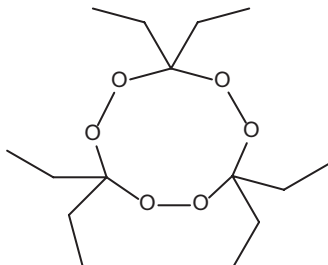
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- [11] J. A. Wyler, *Preparation of Tripentaerythritol Octanitrate*, US Patent 2,389,228, November 20th **1945**.
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Tripentanone triperoxide

Name [German, acronym]: 1,2,4,5,7,8-Hexaoxacyclononane,3,3,6,6,9,9-hexaethyl, 3,3,6,6,9,9-hexaethyl-1,2,4,5,7,8-hexaoxo-nonane, 3,3,6,6,9,9-hexaethyl-1,2,4,5,7,8-hexaoxacyclononane, 1,1,4,4,7,7-hexaethyl-1,4,7-cyclononatriperoxane, diethyl ketone peroxide [TPTP, DEKTP]

Main (potential) use: Possible lower-risk training substitute for TATP

Structural formula:



	TPTP
Formula	$C_{15}H_{30}O_6$
Molecular mass [g mol ⁻¹]	306.40
Appearance at RT	White, needle-like solid ^[1, 3] , colorless needle crystals ^[2]
IS [J]	Fol = <10 (Rotter impact test, 5 kg mass, 30 mg) ^[1, 3]
FS [N]	<5 (BAM) ^[1, 3]
ESD [J]	Initiation @ 4.5 but not @ 0.45 J (DSTO apparatus) ^[1, 3]
N [%]	0.00
$\Omega(CO_2)$ [%]	-203.66
$T_{m.p.}$ [°C]	332 ^[2]
$T_{dec.}$ [°C]	
ρ [g cm ⁻³]	1.115 (crystal @ 296 K, X-ray) ^[2]
Heat of formation	

	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^\circ$ [kJ kg ⁻¹]			
T_{ex} [K]			
$p_{\text{C-J}}$ [kbar]			
VoD [m s ⁻¹]			
V_0 [L kg ⁻¹]			
5 s explosion T [°C] Ignition T [°C]	153 (violent explosion) ^[1, 3]		
Thermal stability	Less stable than TATP in soln. ^[3]		
Volatility	Extremely slow sublimation @ RT: <1 mg weight loss in sample left open to atmosphere @ ambient T for 30 days ^[3] , no sublimation observed on drying in vacuo @ ~ 1 mbar @ RT for 12 h ^[3]		
Solubility [g/mL]	Soluble in warm MeOH ^[3] , NMR recorded in CDCl ₃ ^[3]		
Hygroscopicity	Samples remained as loose crystalline powders after string at ambient conditions ^[3]		
Compatibility	Degraded by hydrochloric acid ^[3]		
	Relatively stable @ RT to many reducing agents ^[3] :		
	Compound	Degradation	Compound
	Molybdenum hydrogen bronze	N	ZnS
	Cu(I) Cl.Neocuproine ₂	N	K ₃ Fe(CN) ₆
	Cu(II)Salen	N	Na ₂ SO ₃
	Sc ₂ (SO ₄) ₃	N	Na ₂ S ₂ O ₃
	FeCl ₂	N	<i>p</i> -Aminophenol
	CuCl ₂	N	Diethylenetriamine
	MnO ₂	N	Triphenylphosphine
	MnCl ₂	N	Hydroquinone
	Zn powder	N	<i>p</i> -Tolyldiazine hydrochloride

	Co(NO ₃) ₂	N	Hydroxylamine hydrochloride	N
	Li ₂ B ₄ O ₇	N	Thiourea	N
	Ethanox 330	N	Ferrocene	N
	Antioxidant 425	N	B(OH) ₃	N
	Montmorillonite K10	N	<i>p</i> -Quinone dioxime	N
	Montmorillonite K10.ammonia	N	Semicarbazide hydrochloride	N
	TiO ₂	N	Trimethyl phosphite	N
	ZnCl ₂	N		

	Diethyl ketone peroxide ^[2]
Chemical formula	C ₁₅ H ₃₀ O ₆
Molecular weight [g mol ⁻¹]	306.39
Crystal system	Monoclinic
Space group	<i>P</i> 2 ₁ / <i>c</i>
<i>a</i> [Å]	10.4545(12)
<i>b</i> [Å]	10.859(3)
<i>c</i> [Å]	32.168(5)
<i>α</i> [°]	90
<i>β</i> [°]	91.796(10)
<i>γ</i> [°]	90
<i>V</i> [Å ³]	3,650.0(12)
<i>Z</i>	8
<i>ρ</i> _{calc} [g cm ⁻³]	1.115
<i>T</i> [K]	296

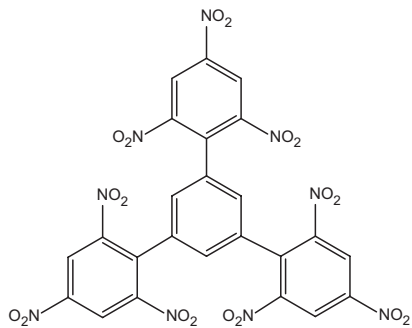
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1,3,5-Tripicrylbenzene

Name [German, acronym]: 1,3,5-Tripicrylbenzene, tripicrylbenzene, 2-[3,5-bis(2,4,6-trinitrophenyl)phenyl]-1,3,5-trinitrobenzene [TNTPB, TPB]

Main (potential) use: Detonator, primary explosive; secondary explosive patented for use in booster cups and exploding bridge wire EBW) detonators^[4]

Structural formula:



	1,3,5-Tripicrylbenzene
Formula	C ₂₄ H ₉ N ₉ O ₁₈
Molecular mass [g mol ⁻¹]	711.38
Appearance at RT	
IS [J]	
FS [N]	
ESD [J]	
N [%]	17.72
Ω(CO ₂) [%]	-77.60
T _{m,p.} [°C]	386 ^[1]
T _{phase transition} [°C]	215 (endotherm, DTA) ^[4]
T _{dec.} [°C]	>400 (crude product) ^[4] , 372 (exotherm, DTA, recryst.) ^[4]
ρ [g cm ⁻³]	1.670 ^[3]
Heat of formation	-62.1 kcal mol ⁻¹ (static bomb calorimetry) ^[3] , -62.1 (standard heat of formation, ΔH _f ^o) ^[5]
Heat of combustion	-2,502.6 kcal mol ⁻¹ (Δ _c H ^o , static bomb calorimetry) ^[3] , -2,501.6 kcal/mol (standard heat of combustion, ΔH _c ^o) ^[5]

	Calcd. (EXPLOS 6.04)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^\circ$ [kJ kg ⁻¹]			
T_{ex} [K]		2,877 (units not specified) (@ 1.67 g cm ⁻³ , BKW TNT param.) ^[6]	
p_{CJ} [kbar]		187 (calcd., K-J) ^[3] 197 (@ 1.67 g cm ⁻³ , BKW RDX param.) ^[6] 189 (@ 1.67 g cm ⁻³ , BKW TNT param.) ^[6]	
VoD [m s ⁻¹]		6,640 (@ 1.670 g cm ⁻³ , calcd. K-J) ^[3] 6,896 (@ 1.67 g cm ⁻³ , BKW RDX param.) ^[6] 6,646 (@ 1.67 g cm ⁻³ , BKW TNT param.) ^[6]	
V_0 [L kg ⁻¹]			
Brisance	% brisance with hours @ 500°F: 96% @ 100 h, 90% @ 200 h, 71% @ 300 h, 40% @ 400 h ^[4]		
Gap test	50% card gap = 30 cards ^[4]		
Vacuum stability test [cm ³ /days]	@ 200 °C: 0.1/2, 0.1/7, 0.2/14, 0.2/21, 0.3/28, 0.3/35, 0.3/42, 0.4/49, 0.4/56, 0.4/63, 0.5/70, 3.2/77, 7.0/84, 9.5/91 ^[2] @ 175 °C: 0.1/2, 0.1/7, 0.1/14, 0.1/21, 0.1/28, 0.1/35, 0.2/42, 0.2/49, 0.2/56, 0.2/63, 0.2/70, 0.2/77, 0.3/84, 0.3/91 ^[2]		
Solubility [g/mL]	Soluble in acetone ^[4]		

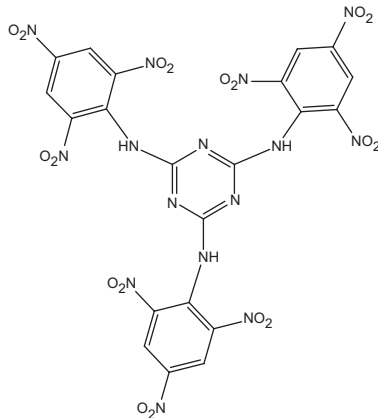
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*N*²,*N*⁴,*N*⁶-Tripicrylmelamine

Name [German, acronym]: Tripicrylmelamine, *N,N',N''*-tripicrylmelamine, 2,4,6-tris-picrylamino-*s*-triazine [TPM]

Main (potential) use: Patented for possible use as heat-resistant explosive^[1]

Structural formula:



	Tripicrylmelamine
Formula	C ₂₁ H ₉ N ₁₅ O ₁₈
Molecular mass [g mol ⁻¹]	759.39
Appearance at RT	Crystalline solid ^[9]
IS [J]	Insensitive ^[1] , 320 cm (2.5 kg mass) ^[1] , 200 cm ^[4] , 200 cm (2.5 kg mass, type 12 apparatus cf. <i>H</i> _{50%} = 156 cm for TNT) ^[6] , <i>H</i> _{50%} = 37 cm (5 kg mass, sandpaper, type 12 apparatus) ^[6] , <i>H</i> _{50%} = 54 cm (AFX-511: 95 wt.% TPM, 5 wt.% Kel-F 800 @ 1.69 g cm ⁻³ (96.5% TMD); 5 kg mass, sandpaper, type 12 apparatus) ^[6] , 320 cm ^[9] , <i>H</i> ₅₀ ≥ 320 cm (type 12, ERL apparatus) ^[10] , <i>H</i> ₅₀ ≥ 320 cm (type 12B, ERL apparatus) ^[10] , <i>H</i> ₅₀ = 161 ± 0.25 cm (type 12B, ERL apparatus) ^[10]
FS [N]	Inert over the range of the LASL friction test ^[6]
<i>N</i> [%]	27.67
Ω(CO ₂) [%]	-60.04
<i>T</i> _{m.p.} [°C]	316 ^[4] , 316 (dec.) ^[6] , >300 (dec.) ^[9]
<i>T</i> _{dec.} [°C]	325 (exotherm, DTA) ^[1, 9] , 300 (DTA) ^[4, 6] , 290 (slow onset of exo) 316 (melting endo), rapid dec. after TPM melts (DTA @ 20 °C/min) ^[6] , stable to 290 °C (DTA @ 20 °C/min) ^[6] , 601.4 K (DSC) ^[8]
ρ [g cm ⁻³]	1.75 (crystal) ^[1] , 1.74 (crystal) ^[4, 6] , 1.75 ^[9]

Heat of formation															
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.												
$-\Delta_{\text{ex}}U^{\circ}$ [kJ kg ⁻¹]															
T_{ex} [K]															
$p_{\text{C-J}}$ [kbar]		240 (@ 1.75 g cm ⁻³ , calcd.) ^[1] 23.8 GPa ^[4, 6]													
VoD [m s ⁻¹]		7,420 (@ 1.75 g cm ⁻³ , calcd.) ^[1] 7,420 (@ crystal density, calcd.) ^[6]	7,180 (AFX-511: 95 wt.% TPM, 5 wt.% Kel-F 800 @ 1.69 g cm ⁻³ (96.5% TMD)) ^[6] 7,400 (AFX-511: 95 wt.% TPM, 5 wt.% Kel-F 800; value obtained by extrapolating to 100% TMD) ^[6]												
V_0 [L kg ⁻¹]															
Critical T [°C]	316 ± 2 (ρ = 1.66 g cm ⁻³) ^[10]														
SSGT [cm]	LASL SSGT on AFX-511: 95 wt.% TPM, 5 wt.% Kel-F 800 @ 1.69 g cm ⁻³ (96.5% TMD) ^[6] ; 50% point = 0.63 mm (cf. 0.33 mm for TNT @ 1.633 g cm ⁻³) ^[6]														
Thermal stability	No physical changes in neat sample observed up to 250 °C and no EPR signal observed ^[7]														
Vacuum stability test [cm ³ /h]	@ 200 °C, terminated after 27 days, total gas evolved (cm ³ /g) @ STP, residue = darker than original sample, moderate amount of sublimate ^[2] : <table><tr><td>Gas evolved (cm³/g)</td><td>Time of exposure (days)</td></tr><tr><td>0.8</td><td>2</td></tr><tr><td>4.2</td><td>7</td></tr><tr><td>7.7</td><td>14</td></tr><tr><td>11.7</td><td>21</td></tr><tr><td>15.6</td><td>28</td></tr></table>			Gas evolved (cm ³ /g)	Time of exposure (days)	0.8	2	4.2	7	7.7	14	11.7	21	15.6	28
Gas evolved (cm ³ /g)	Time of exposure (days)														
0.8	2														
4.2	7														
7.7	14														
11.7	21														
15.6	28														

	<p>@ 175 °C, total gas evolved (cm³/g) @ STP, residue darker than original sample, no sublimate detected visibly^[2, 5]:</p> <table><tr><th>Gas evolved (cm³/g)</th><th>Time of exposure (days)</th><th>Gas evolved (cm³/g)</th><th>Time of exposure (days)</th></tr><tr><td>1.5</td><td>2</td><td>4.1</td><td>49</td></tr><tr><td>2.0</td><td>7</td><td>4.5</td><td>56</td></tr><tr><td>2.3</td><td>14</td><td>4.9</td><td>63</td></tr><tr><td>2.6</td><td>21</td><td>5.2</td><td>70</td></tr><tr><td>2.9</td><td>28</td><td>5.5</td><td>77</td></tr><tr><td>3.3</td><td>35</td><td>5.9</td><td>84</td></tr><tr><td>3.7</td><td>42</td><td>6.7</td><td>91</td></tr></table> <p>@ 150 °C, total gas evolved (cm³/g) @ STP, not much change in residue from original sample, no sublimate detected visibly^[2]:</p> <table><tr><th>Gas evolved (cm³/g)</th><th>Time of exposure (days)</th><th>Gas evolved (cm³/g)</th><th>Time of exposure (days)</th></tr><tr><td>1.0</td><td>2</td><td>1.3</td><td>49</td></tr><tr><td>1.1</td><td>7</td><td>1.3</td><td>56</td></tr><tr><td>1.1</td><td>14</td><td>1.3</td><td>63</td></tr><tr><td>1.2</td><td>21</td><td>1.3</td><td>70</td></tr><tr><td>1.2</td><td>28</td><td>1.4</td><td>77</td></tr><tr><td>1.2</td><td>35</td><td>1.4</td><td>84</td></tr><tr><td>1.2</td><td>42</td><td>1.5</td><td>91</td></tr></table> <p>0.8 cm³/g/48 h @ 200 °C^[6], 1.5 cm³/g/91 days @ 150 °C^[6], 0.07 cm³/g/48 h @ 120 °C (AFX-511: 95 wt.% TPM, 5 wt.% Kel-F 800 @ 1.69 g cm⁻³ (96.5% TMD))^[6]</p>	Gas evolved (cm ³ /g)	Time of exposure (days)	Gas evolved (cm ³ /g)	Time of exposure (days)	1.5	2	4.1	49	2.0	7	4.5	56	2.3	14	4.9	63	2.6	21	5.2	70	2.9	28	5.5	77	3.3	35	5.9	84	3.7	42	6.7	91	Gas evolved (cm ³ /g)	Time of exposure (days)	Gas evolved (cm ³ /g)	Time of exposure (days)	1.0	2	1.3	49	1.1	7	1.3	56	1.1	14	1.3	63	1.2	21	1.3	70	1.2	28	1.4	77	1.2	35	1.4	84	1.2	42	1.5	91
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Solubility [g/mL]	Soluble in acetone ^[1, 6] , recryst. from CH ₃ CN/EtOH ^[1] , soluble in THF ^[6] , less soluble in methyl ethyl ketone and ethyl acetate ^[6]																																																																
Compatibility	50/50 mixture of TPM and TNT showed a characteristic but accelerated TNT EPR spectrum after ~ 3 min @ 168 °C ^[7]																																																																
ΔH _{dec} [J/g]	Q _{dec} = 3,366 kJ/mol (DSC) ^[8]																																																																
Plate dent test [mm]	3.40 (AFX-511: 95 wt.% TPM, 5 wt.% Kel-F 800 @ 1.69 g cm ⁻³ (96.5% TMD, 1.27 cm diameter, confined) ^[6]																																																																
Thermal conductivity [cal/cm-s-°C]	5 × 10 ⁻⁴ (@ density = 1.75 g cm ⁻³) ^[10]																																																																

Large TPM crystals can be obtained by diluting a saturated soln. of TPM in acetone with an equal volume of MeOH followed by slow evaporation of the solvents.^[6]

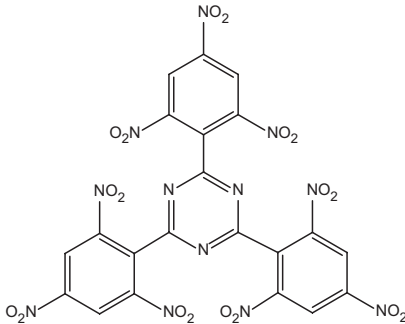
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2,4,6-Tripicryl-s-triazine

Name [German, acronym]: 2,4,6-Tripicryltriazine, 2,4,6-tris(2,4,6-trinitrophenyl)-1,3,5-triazine [TPT, TPTA]

Main (potential) use: Patented as a thermally stable explosive^[4], component of perforators or detonators in downhole well applications, possible spacecraft applications^[6], possible thermally stable explosive^[12], heat resistant explosive with promise for use in mild detonating cords and flexible liner-shaped charges^[13]

Structural formula:



	2,4,6-Tripicryl-s-triazine																	
Formula	C ₂₁ H ₆ N ₁₂ O ₁₈																	
Molecular mass [g mol ⁻¹]	717.42																	
Appearance at RT	Pale yellow crystalline solid ^[4] , white crystalline solid ^[13] , bright yellow crystals if acetone solvent of crystallization present ^[13]																	
IS [J]	320 cm (2.5 kg mass) ^[2] , 93 cm ^[4] , 22.85 (Bruceton) ^[7, 10] , H _{50%} = 74 cm (2.5 kg mass, type 12 tool, sandpaper) ^[12]																	
ESD [J]	20 consecutive shots with no smoke, burning and/or explosion @ 10 K Volt potential, 0.0 mFD capacitance ^[12] Max. no fire values for capacitance/voltage level, data from ^[12] : <table><tr><th rowspan="2">Cap. (mfd)</th><th colspan="2">TPT</th></tr><tr><th>m/m</th><th>m/r</th></tr><tr><td>1.0</td><td>4,500</td><td>–</td></tr><tr><td>0.1</td><td>4,500</td><td>4,000</td></tr><tr><td>0.01</td><td>7,500*</td><td>6,500</td></tr><tr><td>0.001</td><td>7,500*</td><td>7,500*</td></tr></table>	Cap. (mfd)	TPT		m/m	m/r	1.0	4,500	–	0.1	4,500	4,000	0.01	7,500*	6,500	0.001	7,500*	7,500*
Cap. (mfd)	TPT																	
	m/m	m/r																
1.0	4,500	–																
0.1	4,500	4,000																
0.01	7,500*	6,500																
0.001	7,500*	7,500*																

N [%]	23.53		
$\Omega(\text{CO}_2)$ [%]	-63.53		
$T_{\text{m.p.}}$ [°C]	352–353 ^[2, 3, 7, 8] , 352 ^[3, 8, 12] , 349–351 ^[3, 8] , 350–351 (cryst., dec.) ^[4] , 352–353 (cryst., high purity, dec.) ^[4] , 349–351 (crystals obtained from <i>m</i> -dinitrobenzene @ 200 °C) ^[13]		
$T_{\text{dec.}}$ [°C]	319.6–320.4 (onset, DTA, (s)) ^[7] , 340 (DTA, onset, exotherm) ^[10] , 320 (DTA, onset exotherm) ^[10] , 359 (onset, DTA) ^[7]		
ρ [g cm ⁻³]	1.67 (crystal) ^[1] , 1.75 (TMD) ^[2] , 1.724 (recryst.) ^[2] , 1.67 (crystals obtained from acetone which are heated to remove solvent of cryst.) ^[13] , 1.724 (average value using lead perchlorate solns.) ^[13] , 1.637 (TPT-acetone solvate, crystals from acetone/MeOH, lead perchlorate soln.) ^[13]		
Heat of formation	73.2 kcal/mol ^[1] , 7.56 kcal mol ⁻¹ (combustion calorimetry) ^[5] , 7.56 + 0.99 kcal/mol (ΔH_f° , combustion calorimetry) ^[14] , 70.87 ± 1.68 kcal/mol (enthalpy of form., Pt-lined bomb calorimeter) ^[15]		
Heat of combustion	-2,253.2 kcal mol ⁻¹ ^[1] , -2,256 kcal/mol ^[2]		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^\circ$ [kJ kg ⁻¹]		4,324 MJ•kg ⁻¹ (Q_{real}) ^[7] 4,324 MJ•kg ⁻¹ (Q_{real} , calcd., semi-empirical Pepekkin method) ^[10]	
T_{ex} [K]			
$p_{\text{C-1}}$ [kbar]		212 (calcd., K-J) ^[1]	
VoD [m s ⁻¹]		7,080 (@ 1.67 g cm ⁻³ , calcd. K-J) ^[1] 7,080 (@ TMD, calcd., K-J) ^[7, 10]	7,420 (@ 1.75 g cm ⁻³) ^[2] ~5,500 (@ ~1.15 g cm ⁻³ , 0.2 in column diameter, values est. from graph) ^[12] ~5,950 (@ ~1.28 g cm ⁻³ , 0.2 in column diameter, values est. from graph) ^[12] ~5,850 (@ ~1.28 g cm ⁻³ , 0.2 in column diameter, values est. from graph) ^[12] ~6,550 (@ ~1.48 g cm ⁻³ , 0.2 in column diameter, values est. from graph) ^[12]

			<p>~7,050 (@ ~ 1.68 g cm⁻³, 0.2 in column diameter, values est. from graph)^[12]</p> <p>~5,700 (@ ~ 1.30 g cm⁻³, 0.1 in column diameter, values est. from graph)^[12]</p> <p>~6,000 (@ ~ 1.33 g cm⁻³, 0.1 in column diameter, values est. from graph)^[12]</p> <p>~7,050 (@ ~ 1.65 g cm⁻³, 0.1 in column diameter, values est. from graph)^[12]</p> <p>~7,000 (@ ~ 1.70 g cm⁻³, 0.1 in column diameter, values est. from graph)^[12]</p> <p>~6,250 (@ ~ 1.40 g cm⁻³, 0.3 in column diameter, values est. from graph)^[12]</p> <p>~6,900 (@ ~ 1.58 g cm⁻³, 0.3 in column diameter, values est. from graph)^[12]</p> <p>~7,050 (@ ~ 1.70 g cm⁻³, 0.3 in column diameter, values est. from graph)^[12]</p>																																																			
V ₀ [L kg ⁻¹]																																																						
SSGT [cm]	TPT shock sensitivity similar to that of HNS, data from ^[12] :																																																					
	<table><tr><th rowspan="2">Loading pressure (kpsi)</th><th colspan="2">Density (g/cm³)</th><th colspan="4">Sensitivity (DBG)</th></tr><tr><th>Avg.</th><th>s</th><th>Avg</th><th>g</th><th>s_m</th><th>N</th></tr><tr><td>4</td><td>1.193</td><td>0.0557</td><td>4.800</td><td>0.0414</td><td>0.0281</td><td>20</td></tr><tr><td>8</td><td>1.242</td><td>0.0214</td><td>4.753</td><td>0.0312</td><td>0.0205</td><td>20</td></tr><tr><td>16</td><td>1.325</td><td>0.0496</td><td>5.059</td><td>0.0384</td><td>0.0257</td><td>20</td></tr><tr><td>32</td><td>1.444</td><td>0.0268</td><td>5.423</td><td>0.0798</td><td>0.0430</td><td>20</td></tr><tr><td>64</td><td>1.658</td><td>0.0111</td><td>7.217</td><td>0.0988</td><td>0.0530</td><td>20</td></tr></table>						Loading pressure (kpsi)	Density (g/cm ³)		Sensitivity (DBG)				Avg.	s	Avg	g	s _m	N	4	1.193	0.0557	4.800	0.0414	0.0281	20	8	1.242	0.0214	4.753	0.0312	0.0205	20	16	1.325	0.0496	5.059	0.0384	0.0257	20	32	1.444	0.0268	5.423	0.0798	0.0430	20	64	1.658	0.0111	7.217	0.0988	0.0530	20
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5 s explosion T [°C] Ignition T [°C]	350–360 ^[7, 10] , 359 (lit. cited in ^[7, 10])																																			
Thermal stability	283 (threshold of thermal stability) ^[7, 10]																																			
Vacuum stability test [cm ³ /h]	<p>0.4/g/h @ 300 °C (for 2 h period)^[4] @ 200 °C, total gas evolved (cm³/g) @ STP/time of exposure (days)^[9, 11]: 0.2/2, 0.2/7, 0.4/14, 0.4/21, 0.4/28, 0.4/35, 0.5/42, 0.5/49, 0.6/56, 0.7/63, 0.9/70, 1.0/77, 1.0/84, 1.1/91^[9, 11]</p> <p>Data from^[12]:</p> <table><tr><td>T (°C)</td><td>20 min surge (cc/g)</td><td>2 h period (cc/g/h)</td></tr><tr><td>280</td><td>0.29</td><td>0.10</td></tr><tr><td>300</td><td>0.37</td><td>0.29</td></tr><tr><td>315</td><td>0.50</td><td>1.20</td></tr></table> <p>@ 278 °C, 16 h, 97.1% TPT in residue after heat treatment under vacuum^[12], @ 250 °C, 44 h, 99.3% TPT in residue after heat treatment under vacuum^[12]</p>	T (°C)	20 min surge (cc/g)	2 h period (cc/g/h)	280	0.29	0.10	300	0.37	0.29	315	0.50	1.20																							
T (°C)	20 min surge (cc/g)	2 h period (cc/g/h)																																		
280	0.29	0.10																																		
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Vapor pressure [atm. @ °C]	<p>Data from^[12]:</p> <table><tr><td>T (°C)</td><td>Δt (s)</td><td>Surface area (cm²)</td><td>Wt. loss (g)</td><td>Vapor pressure (Torr)</td></tr><tr><td>277.8</td><td>55,500</td><td>6.3</td><td>0.1268</td><td>4.77(10⁻⁶)</td></tr><tr><td>247.6</td><td>157,380</td><td>5.1</td><td>0.0227</td><td>4.26(10⁻⁷)</td></tr><tr><td>247.6</td><td>236,100</td><td>5.1</td><td>0.0303</td><td>3.70(10⁻⁷)</td></tr><tr><td>206.9</td><td>239,400</td><td>5.1</td><td>0.0024</td><td>2.73(10⁻⁸)</td></tr><tr><td>206.9</td><td>768,900</td><td>5.1</td><td>0.0041</td><td>1.48(10⁻⁸)</td></tr><tr><td>98.9</td><td>149,040</td><td>5.1</td><td colspan="2">Indeterminate</td></tr></table>	T (°C)	Δt (s)	Surface area (cm ²)	Wt. loss (g)	Vapor pressure (Torr)	277.8	55,500	6.3	0.1268	4.77(10 ⁻⁶)	247.6	157,380	5.1	0.0227	4.26(10 ⁻⁷)	247.6	236,100	5.1	0.0303	3.70(10 ⁻⁷)	206.9	239,400	5.1	0.0024	2.73(10 ⁻⁸)	206.9	768,900	5.1	0.0041	1.48(10 ⁻⁸)	98.9	149,040	5.1	Indeterminate	
T (°C)	Δt (s)	Surface area (cm ²)	Wt. loss (g)	Vapor pressure (Torr)																																
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98.9	149,040	5.1	Indeterminate																																	
Solubility [g/mL]	Recryst. from acetone or acetone/MeOH, <i>m</i> -dinitrobenzene ^[13] , TLC performed in C ₆ H ₆ ^[8] , NMR recorded in DMSO ^[8]																																			

Bright yellow crystals obtained by recryst. from acetone or acetone/MeOH solns. are 1:1 solvates with acetone, solvent of crystallization can be removed by heating crystals @ $T \geq 140$ °C which produces opaque, white solid^[13]

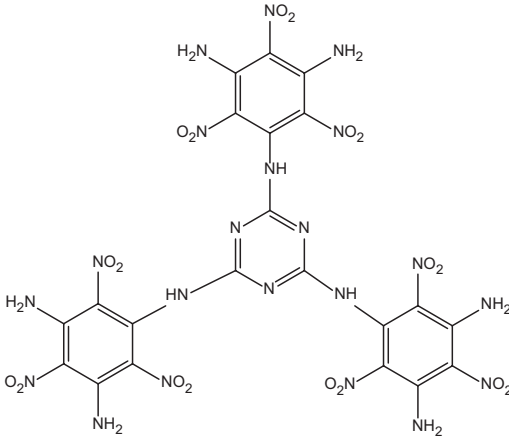
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2,4,6-Tris(3',5'-diamino-2',4',6'-trinitrophenylamino)-1,3,5-triazene

Name [German, acronym]: 2,4,6-Tris(3,5-diamino-2,4,6-trinitrophenylamino)-1,3,5-triazine [PL-1]

Main (potential) use: Thermally stable, insensitive explosive^[1]

Structural formula:



	PL-1
Formula	$C_{21}H_{15}N_{21}O_{18}$
Molecular mass [g mol ⁻¹]	849.48
Appearance at RT	Yellow solid ^[3]
IS [J]	170 cm ^[2] , $H_{50\%} = 170$ cm (2 kg mass) ^[3]
FS [N]	≈36 kg (Julius-Peters apparatus) ^[3]
N [%]	34.63
Ω(CO ₂) [%]	-59.36
$T_{m.p.}$ [°C]	336 ^[2] , 336 (dec., @ 2 °C/min, uncorrected) ^[3] , ~ 336 ^[1, 7]
$T_{dec.}$ [°C]	336 (@ 2 °C/min, uncorrected) ^[3] , 335 (DSC @ 10 °C/min) ^[3] , 325 (T_i), 335 (T_m) (DTA, exotherm) ^[3] , 338.7 (DTA @ 5 °C/min) ^[3] , 348.7 (DTA @ 10 °C/min) ^[3] , 355.1 (DTA @ 15 °C/min) ^[3] , 360.3 (DTA @ 20 °C/min) ^[3] , 363.5 (DTA @ 25 °C/min) ^[3] , 335 (DTA @ 10 °C/min) ^[5]
ρ [g cm ⁻³]	2.02 ^[1, 2, 5] , 2.02 (density bottle method) ^[3] , 2.02 (crystal) ^[6] , 1.893 (calcd., <i>EDPHT 2.0</i>) ^[6] , 1.840 (calcd., <i>Ammon</i>) ^[6] , ~ 2.02 ^[7]
Heat of formation	427.6 kJ/mol (calcd., isodesmic) ^[4] , 24.2 kcal/mol (condensed phase, calcd. empirical method) ^[5] , 225 kcal/mol (gas-phase heat of form., calcd.) ^[5]

	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^{\circ}$ [kJ kg ⁻¹]		Heat of det. = 2.5 kJ/g (calcd.) ^[5]	
T_{ex} [K]		3,467 (calcd.) ^[5]	
$p_{\text{C-J}}$ [kbar]		312 (@ 2.02 g cm ⁻³ , calcd.) ^[3] 35.5 GPa (based on heat of form. = 427.6 kJ/mol, calcd., K-J) ^[4] 307 (based on predicted heat of form. of 27.2 kcal/mol, calcd., empirical method) ^[5]	
VoD [m s ⁻¹]		7,861 (@ 2.02 g cm ⁻³ , calcd.) ^[3] 8,500 (based on heat of form. = 427.6 kJ/mol, calcd., K-J) ^[4]	
V_0 [L kg ⁻¹]			
SSGT [cm]	$P_{90} = 86.6$ kbar (calcd., @ 90% TMD) ^[5] , $P_{95} = 132.9$ kbar (calcd., @ 95% TMD) ^[5] , $P_{99} = 168.3$ kbar (calcd., @ 90% TMD) ^[5]		
Solubility [g/mL]	Poorly soluble in organic solvents ^[3]		

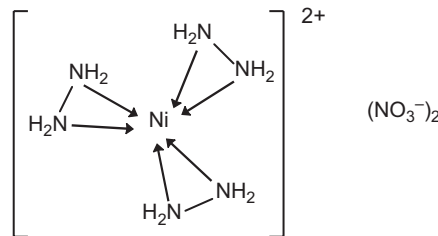
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Tris-hydrazinenickel(II) nitrate

Name [German, acronym]: Nickel hydrazine nitrate, nickel hydrazinium nitrate [nickelhydrazinnitrat, NHN, NiHN]

Main (potential) use: Possible future Pb-free primary explosive^[1, 4, 7], possible applications in smoke-free fireworks^[2], possible future replacement for LA as an intermediate charge in commercial detonators^[5], investigated as potential component of squib compositions for igniting propellants and explosives^[7], possible future safe alternative to LS and possible partial replacement for LA^[8]

Structural formula:



	NiHN
Formula	$\text{H}_{12}\text{N}_8\text{NiO}_6$
Molecular mass [g mol ⁻¹]	278.84
Appearance at RT	Purple-colored solid ^[7] , purple-violet solid ^[10] , pink, square crystals ^[8]
IS [J]	Equivalent to that of LA ^[1] , 96 cm ^[4] , 26 cm (100% fire height); 21 cm (100% no-fire height) (400 g hammer, 20 mg sample) ^[5] , 9 cm (ball drop, 500 g, 50% explosion) ^[6] , $H_{50\%} = 84$ cm ^[7] , 21 cm (400 g mass, 20 mg sample, 50% explosion) ^[10] , $H_{50\%} = 96$ cm (2 kg mass) ^[8]
FS [N]	Same as that of AgN_3 ^[1] , 1 kg ^[4] , 12% (explosion percentage of 25 samples under 588.40 kPa and 80° swing angle) ^[5] , insensitive up to 10 N ^[7] , 1.6 kg ^{f[10]} , 1.0 kg (friction insensitiveness) ^[8]
ESD [J]	Same as that of AgN_3 ^[1] , 5 (spark insensitivity) ^[4, 8] , 0.02 (minimum energy) ^[5] , 0.02 ^[10]
N [%]	40.18
$\Omega(\text{CO}_2)$ [%]	
$T_{m.p.}$ [°C]	

$T_{\text{dec.}}$ [°C]	220 (onset, DTA/TG) ^[1] , 232 (DTA) ^[2] , 247–259 (NHN coated with WPU, DTA) ^[2] , 220 (DTA @ 10 °C/min, air, Pt cup, 10 mg sample) ^[6] , 210 (exo, onset), 220 (exo, peak max) (DSC @ 5 °C/min) ^[7] , 215–235 (rapid mass loss, total mass loss = 92.5%, TG) ^[7] , 220 (violent reaction followed by explosion, DSC) ^[7] , 505.7 K (onset), 506.5 K (peak) (rapid single-stage exothermic dec.) ^[10]																						
ρ [g cm ⁻³]	<p>2.129^[1], 1.55 (pressed under 20–40 MPa)^[1], ~ 1.70 (pressed under 60–80 MPa)^[1], 2.129 (@ 25 °C, pycnometric method in 95% EtOH)^[5], 0.85 – ~ 0.95 (free ρ, volumetric method)^[5], 0.85–0.90 (bulk ρ)^[7], 2.1 (crystal ρ)^[10], 2.12^[10], 1.2 (bulk density, after addition of additives such as 1% dextrin and dioctyl succinate during synthetic process)^[8], 0.85–0.90 (bulk density without additives)^[8]</p> <p>Pressure/density curve values^[5]:</p> <table><tr><td>P (MPa)</td><td>0</td><td>20</td><td>40</td><td>60</td><td>80</td></tr><tr><td>ρ (g/cm³)</td><td>0.9108</td><td>1.5464</td><td>1.5631</td><td>1.6984</td><td>1.7133</td></tr><tr><td>Σ</td><td>0.0194</td><td>0.0054</td><td>0.0096</td><td>0.0077</td><td>0.0056</td></tr></table>					P (MPa)	0	20	40	60	80	ρ (g/cm ³)	0.9108	1.5464	1.5631	1.6984	1.7133	Σ	0.0194	0.0054	0.0096	0.0077	0.0056
P (MPa)	0	20	40	60	80																		
ρ (g/cm ³)	0.9108	1.5464	1.5631	1.6984	1.7133																		
Σ	0.0194	0.0054	0.0096	0.0077	0.0056																		
Heat of formation	–449 kJ/mol (exptl. value) ^[10]																						
Heat of combustion	5,225 kJ/kg (exptl. value) ^[10]																						
	Calcd. (EXPLOS 6.03)	Lit. values		Exptl.																			
$-\Delta_{\text{ex}}U^{\circ}$ [kJ kg ⁻¹]				Q_{ex} = 1,014 cal/g (in 1 atm. air) ^[5] Heat of explosion = 4,390 kJ/kg ^[10]																			
T_{ex} [K]		2,342 (theoretical value) ^[10]																					
$p_{\text{C-J}}$ [kbar]		20.8 GPa (theoretical value, @ 1.7 g cm ⁻³) ^[10]																					
VoD [m s ⁻¹]		7,000 (@ 1.7 g cm ⁻³) ^[10]		7,000 (@ 1.7 g cm ⁻³) ^[1, 5] 3,600 (@ tap density of 0.8 g cm ⁻³ , flash X-ray technique) ^[8] 6,900 (loading density of 1.7 g cm ⁻³ after consolidation under 150 MPa pressure) ^[8]																			

V_0 [L kg ⁻¹]	884 (theoretical value) ^[10]												
Initiation ability	<p>0.15 g (minimal charge in a No. 8 detonator toward PETN)^[1], 150 mg (minimum priming charge to PETN under the initiating of safety fuse and 120 mg of Nonel's tube (quantity of NHN used as initial charge, minimum priming charge test: 30 MPa to NHN, 15 MPa to PETN booster charge))^[5]</p> <p>NHN with different water ratios initiated directly using blasting caps^[5]:</p> <table> <tr> <th>Water ratio (%)</th><th>Explosion (%)</th></tr> <tr> <td>40</td><td>0</td></tr> <tr> <td>35</td><td>20</td></tr> <tr> <td>25</td><td>80</td></tr> </table> <p>NHN washed with EtOH and then sucked to dryness on filter could be ignited with safety fuse and deflagrated rapidly^[5]</p>	Water ratio (%)	Explosion (%)	40	0	35	20	25	80				
Water ratio (%)	Explosion (%)												
40	0												
35	20												
25	80												
5 s explosion T [°C] 5 s ignition T [°C] Explosion T [°C]	283 (det.) ^[3] , 167 (20 mg sample, Wood's metal bath, extensive disruption of containing blasting cap) ^[5] ~167 ^[1] 219 (heating rate of 5 °C/min) ^[7] , 219 ^[8]												
Thermal stability	505.7 K (onset, dec.), 506.5 K (peak, dec.) (rapid single-stage exothermic dec.) ^[10] , sudden weight loss (~95%) followed by appearance of flash observed in TG ^[10]												
Burn rate [mm/s]	Burns smoke-free ^[2]												
Solubility [g/mL]	<p>Insoluble in H₂O, EtOH, acetone^[1]</p> <p>Data @ RT from^[5]:</p> <table> <tr> <th>Solvent</th><th>g/100 mL solvent (g)</th></tr> <tr> <td>Water</td><td>< 0.0042</td></tr> <tr> <td>EtOH</td><td>< 0.033</td></tr> <tr> <td>Acetone</td><td>< 0.039</td></tr> <tr> <td>MeOH</td><td>< 0.009</td></tr> <tr> <td>Et₂O</td><td>< 0.010</td></tr> </table>	Solvent	g/100 mL solvent (g)	Water	< 0.0042	EtOH	< 0.033	Acetone	< 0.039	MeOH	< 0.009	Et ₂ O	< 0.010
Solvent	g/100 mL solvent (g)												
Water	< 0.0042												
EtOH	< 0.033												
Acetone	< 0.039												
MeOH	< 0.009												
Et ₂ O	< 0.010												

Hygroscopicity	Nonhygroscopic ^[1] , hydrolytically stable ^[5] , 0.34% (moisture content @ 333 K for 10 min) ^[10] Moisture absorption rate of NHN and coated (WPU) NHN ^[2] : <table><tr><th rowspan="2">Sample</th><th colspan="4">Moisture absorption (%)</th></tr><tr><th>2 h</th><th>4 h</th><th>6 h</th><th>8 h</th></tr><tr><td>NHN</td><td>2.0</td><td>3.7</td><td>5.1</td><td>8.0</td></tr><tr><td>Coated NHN</td><td>2.2</td><td>4.1</td><td>5.2</td><td>8.3</td></tr></table>	Sample	Moisture absorption (%)				2 h	4 h	6 h	8 h	NHN	2.0	3.7	5.1	8.0	Coated NHN	2.2	4.1	5.2	8.3
Sample	Moisture absorption (%)																			
	2 h	4 h	6 h	8 h																
NHN	2.0	3.7	5.1	8.0																
Coated NHN	2.2	4.1	5.2	8.3																
Photosensitivity	Unaffected by sunlight ^[1] , no change in its characteristics on prolonged exposure to sunlight ^[5]																			
Compatibility	Ignited by conc. sulfuric acid ^[1] , full dec. by 10% aq. NaOH ^[1] , compatible with Al, Cu, Fe and stainless steel (no reaction after 8 years @ RT) ^[1] , loses its initiation ability on addition of 40% H ₂ O ^[1] , hydrolytically stable – unaffected by stirring with distilled water for 1 week @ 60 °C ^[5] , gentle dec. with weakly acidic solns. but burns on contact with 96% sulfuric acid ^[5] , reacts mildly with 10% NaOH ^[5] , negligible reactivity @ RT after 8 years in the presence of Al, Fe, stainless steel or Cu ^[5] , burns on action of 96% sulfuric acid @ RT ^[5] , weak sulfuric acid soln. only causes gentle dec. ^[5]																			
ΔH_{dec} [J/g]	241.2 (DTA) ^[2] , 251.6–289.3 (NHN coated by WPU, DTA) ^[2]																			
Flame test	flame sensitivity ≥ 30 cm ^[3]																			
Dead pressing	Overpressing occurs @ $P > \sim 60$ MPa ^[1] , NHN needs to get consolidated @ 30 MPa to produce shockwave and does not get dead pressed @ higher pressures ^[8]																			
Radiation sensitivity	Unaffected by X-ray radiation ^[1] , sensitive to IR radiation – can be ignited by the beam of a pulsed CO ₂ laser with energy density of ~ 12.0 J/cm ^{2[1, 5]} , no change in its characteristics on prolonged exposure to X-ray radiation ^[5]																			
Underwater detonation test	Max. pressure cf. values for classical explosives: $P_{\text{max}} = 83.6\%$ RDX, 105.0% TNT, 84.5% HMX, 83.1% PETN ^[9]																			
Miscellaneous	Pressure of gaseous explosion products = 105% that of TNT of equivalent charge ^[1]																			
Witness plate test	Performance evaluation of NHN in detonator No. 27 (NHN = Nickel hydrazinium nitrate, LA = lead azide, SA = silver azide, ASA composition = service lead azide (SLA, 65%), lead styphnate (LS, 32.5%) and Al (2.5%); * = each experiment was repeated 5 times) ^[8] :																			

	Composition Quantity in mg in ()	Puncture on witness plate* Diameter of the hole (mm)	Remarks
	NHN (150) + LA/SA (200)	9	Initiated
	NHN (175) + LA/SA (175)	9	Initiated
	NHN (200) + LA/SA (150)	9	Initiated
	NHN (225) + LA/SA (125)	9	Initiated
	NHN (250) + LA/SA (100)	9	Initiated
	NHN (275) + LA/SA (75)	9	Initiated
	NHN (300) + LA/SA (50)	9	Initiated
	NHN (325) + LA/SA (25)	9	Initiated
	NHN (350)	No puncture	Dent on witness plate
	NHN (325), LA (25) and Tetryl/PETN (550)	9	Initiated
	ASA composition (standard)	9	Initiated

Explosive trains	Results of functioning of explosive train initiated with NHN based detonator No. 10 (* 16 g RDX/wax perforated booster was assembled in main charge, number of trials carried out in each experiment = 5, in all experiments NHN/BNCP was pressed at 30 MPa and CE was at 10 MPa pressure) ^[8] :																								
	<table><tr><td>Composition Charge wt. (mg)</td><td>*RDX/TNT Charge weight (g)</td><td>Initiation method</td><td>Observation</td></tr><tr><td>NHN:CE 350:550</td><td>700</td><td>Safety fuse</td><td>Explosive train</td></tr><tr><td>NHN:CE 350:550</td><td>300</td><td>Safety fuse</td><td>Functioned</td></tr><tr><td>NHN:CE 500:400</td><td>300</td><td>LFCN based General squib</td><td>Witness plate damaged</td></tr><tr><td>NHN 900</td><td>300</td><td>Safety fuse</td><td></td></tr><tr><td>NCP:BNCP:CE 50:300:550</td><td>300</td><td>Safety fuse</td><td>Explosive train functioned, witness plate damaged</td></tr></table>	Composition Charge wt. (mg)	*RDX/TNT Charge weight (g)	Initiation method	Observation	NHN:CE 350:550	700	Safety fuse	Explosive train	NHN:CE 350:550	300	Safety fuse	Functioned	NHN:CE 500:400	300	LFCN based General squib	Witness plate damaged	NHN 900	300	Safety fuse		NCP:BNCP:CE 50:300:550	300	Safety fuse	Explosive train functioned, witness plate damaged
	Composition Charge wt. (mg)	*RDX/TNT Charge weight (g)	Initiation method	Observation																					
	NHN:CE 350:550	700	Safety fuse	Explosive train																					
	NHN:CE 350:550	300	Safety fuse	Functioned																					
	NHN:CE 500:400	300	LFCN based General squib	Witness plate damaged																					
	NHN 900	300	Safety fuse																						
NCP:BNCP:CE 50:300:550	300	Safety fuse	Explosive train functioned, witness plate damaged																						

Effect of different quality of WPU (waterborne polyurethane emulsion) on initiation pressure and 50% sparking distance of the nickel hydrazine nitrate^[2]:

Pressure (MPa)	L_{50} (cm)
55	2.45
190	2.30
225	2.05
310	1.95

Detonation characteristics: relationship between pressure and function^[5]:

Pressure (MPa)	Detonation	Deflagration
<50	5	0
60	5	0
70	3	2
80	2	3

Mean diameter of spheroidal crystals $\geq 80 \mu\text{m}$ ^[1]; coating NHN with WPU does not change the unit cell dimensions^[2], polycrystal crystal shape^[5]

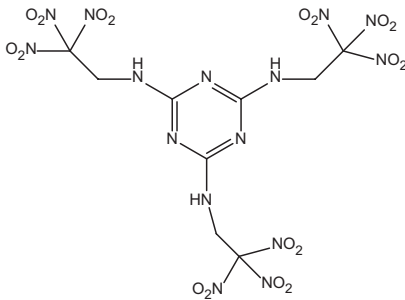
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- [7] J. S. Chhabra, M. B. Talawar, P. S. Makashir, S. N. Asthana, H. Singh, *J. Hazard. Mater.*, **2003**, *A99*, 225–239.
- [8] M. B. Talawar, A. P. Agrawal, J. S. Chhabra, C. K. Ghatak, S. N. Asthana, K. U. B. Rao, *J. Sci. Ind. Res.*, **2004**, *63*, 677–681.
- [9] J. Bełzowski, A. Wojewódka, *Chemik*, **2010**, *64*, 23–24.
- [10] B. Hariharanath, K. S. Chandrabhanu, A. G. Rajendran, M. Ravindran, C. B. Kartha, *Defence Sci. J.*, **2006**, *56*, 383–389.

2,4,6-Tris(2,2,2-trinitroethylamino)-1,3,5-triazine

Name [German, acronym]: 2,4,6-Tris(2,2,2-trinitroethylnitramino)-1,3,5-triazine [TTET]

Main (potential) use: Potential future component of solid rocket fuel compositions^[2]

Structural formula:



	TTET		
Formula	$C_9H_9N_{15}O_{18}$		
Molecular mass [g mol ⁻¹]	615.26		
Appearance at RT	Orange solid ^[1]		
IS [J]	21.5 (Bruceton method, type 12 tool) ^[1]		
N [%]	34.15		
$\Omega(CO_2)$ [%]	-11.7		
$T_{m.p.}$ [°C]	160 ^[1] , 159–160 ^[2]		
$T_{dec.}$ [°C]	186 ^[1]		
ρ [g cm ⁻³]	1.886 (@ RT, gas pycnometer) ^[1]		
Heat of formation	1,175.90 kJ/mol (molar enthalpy of form., calcd., isodesmic) ^[1]		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{ex}U^o$ [kJ kg ⁻¹]			
T_{ex} [K]			

p_{CJ} [kbar]		37.64 GPa (@ 1.886 g cm ⁻³ , calcd., K-J) ^[1]	
VoD [m s ⁻¹]		9,000 (@ 1.886 g cm ⁻³ , calcd., K-J) ^[1]	
V_0 [L kg ⁻¹]			
Solubility [g/mL]	Soluble in isopropyl alcohol ^[2]		

[1] S. Li, W. Zhang, Y. Wang, X. Zhao, L. Zhang, S. Pang, *J. Energet. Mater.*, **2014**, 32, S33–S40.

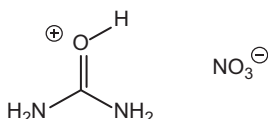
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U

Uronium nitrate

Name [German, acronym]: Uronium nitrate, urea nitrate [harnstoffnitrat, UN]
 Main (potential) use: Improvised explosive, stabilizer in smokeless powders, used in explosive mixtures to lower the explosion temperature

Structural formula:



	Uronium nitrate
Formula	CH ₅ N ₃ O ₄
Molecular mass [g mol ⁻¹]	123.068
Appearance at room temperature (RT)	Solid ^[10] , white monoclinic prisms ^[12] , colorless crystals ^[15]
IS [J]	>40 (500–1,000 μm), ≤49 Nm ^[1, 5] , <i>H</i> ₅₀ >61 inches (Langley one-shot method) ^[6] , insensitive ^[11] , up to 49 Nm without reaction ^[2]
FS [N]	>360 (500–1,000 μm), >353 ^[1] , up to 36 kp pistol load without reaction ^[2]
ESD [J]	>1.5 (500–1,000 μm)
<i>N</i> [%]	34.14
Ω(CO ₂) [%]	–6.50
<i>T</i> _{m.p.} [°C]	155 ^[8] , 140 ^[1] , 157–159 (DSC @ 10 °C/min) ^[3] , 161.5 ^[6] , 152 (dec.) ^[12] , 152.8 (DSC @ 5 °C/min, open alumina cup, dissociation of urea nitrate) ^[13] , 161 (onset, endo), 166 (endo peak max) (DSC @ 20 °C/min) ^[9] , 155 (with dec.) ^[15]
<i>T</i> _{dec.} [°C]	159 (DSC @ 5 °C/min), ~160 (DSC @ 20 °C/min) ^[3] , 157–160 ^[10, 14] , 160 (exo, onset), 172 (exo, peak max) 378 (exo, onset), 409 (exo, peak max) (DSC @ 20 °C/min) ^[9]
ρ [g cm ⁻³]	1.744 (@ 100 K), 1.59 ^[1] , 1.655 (@ 298 K, gas pycnometer), 1.67 ^[3, 10, 14] , 1.50 (under pressure of 1,500 kg/cm ³) ^[11]
Heat of formation	–546.7 kJ/mol (enthalpy of form.) ^[10, 14] , 1,090 kcal/kg (<i>ΔH_f</i>) ^[2] , –562.5 kJ/mol (enthalpy of form., exptl.) ^[19] , –551.0 kJ/mol (enthalpy of form., calcd., emp.) ^[19] , –593.5 kJ/mol (enthalpy of form., calcd., S-D method) ^[19]

Heat of combustion	552.24 kJ/mol ^[10, 14] , 1,071.7 kcal/kg (@ C°) ^[2, 16]	
	Calcd. (EXPLO5 6.03)	Exptl.
$-\Delta_{\text{ex}}U^{\circ}$ [kJ kg ⁻¹]	3,348	639 kcal/kg ^[2] 3,211 [H ₂ O (l)] ^[11] 2,455 [H ₂ O (g)] ^[11]
T_{ex} [K]	2,499	
$p_{\text{C-J}}$ [kbar]	236	
VoD [m s ⁻¹]	7,958	3,400 (@ 0.85 g cm ⁻³ , 30 mm diameter paper tube, driven by 1.5 g MF) ^[2, 9, 11] 4,700 (@ 1.2 g cm ⁻³) ^[15] 4,700 (@ 1.2 g cm ⁻³ , 30 mm steel tube, driven by 1.5 g MF) ^[2, 9, 11]
V_0 [L kg ⁻¹]	916	910 ^[11] 896 ^[2]

Trauzl test [cm ³ , % TNT]	91% TNT ^[7] , 270 cc (10 g UN) comparable sensitivity with that of TNT ^[7] , 260 cm ³ (<i>Kast</i>) ^[11] , 270 cm ³ (<i>Urbanski</i>) ^[11] , 79.6% PA (<i>Médard</i>) ^[11] , 80% PA ^[15] , 272 ^[17] , 270 cc (10 g sample) ^[2]
Ballistic mortar test	92% TNT ^[2, 7]
Initiation efficiency	Incomplete detonation with No. 8 detonator ^[11]
100 °C heat test [% mass loss]	No acid and no explosion in 300 min ^[2] , acid in 30 min but no explosion in 300 min @ 135 °C ^[2]
Thermal stability	0.2% weight loss after 14 days @ 75 °C ^[11] , 1% mass loss after 100 h @ 85 °C ^[15] , satisfactory storage stability when dry ^[2]
Vapor pressure [atm @ °C]	3.94×10^{-5} Pa @ 25 °C ^[8]

Hygroscopicity	Stable, not deliquescent ^[12] , acts corrosively acidic in presence of moisture ^[12] , +0.76% @ 90% RH @ 25 °C ^[2] , +23.2% @ 100% RH, 25 °C ^[2]
Compatibility	Acts corrosively acidic in presence of moisture ^[12]
Heat of melting [J/g]	90 (DSC @ 20 °C/min) ^[9]
Heat of dec. [J/g]	564 (first exotherm, DSC @ 20 °C/min) ^[9] , 634 (second exotherm, DSC @ 20 °C/min) ^[9]
Koenen test	Limiting diameter = <1.0, result = negative ^[18]
Time/pressure test	Maximum pressure >2,070 kPa, time for a pressure rise from 690 to 2,070 kPa = 400 ms ^[18]

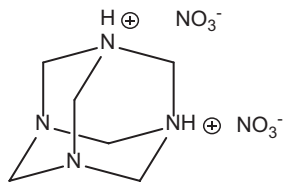
	Urea nitrate ^[4]	Urea nitrate ^[5]
		Neutron diffraction
Chemical formula	CH ₅ N ₃ O ₄	CH ₅ N ₃ O ₄
Molecular weight [g mol ⁻¹]	123.07	123.07
Crystal system	Monoclinic	Monoclinic
Space group	<i>P</i> 2 ₁ / <i>c</i> (no. 14)	<i>P</i> 2 ₁ / <i>c</i> (no. 14)
<i>a</i> [Å]	9.527(7)	9.543(1)
<i>b</i> [Å]	8.203(5)	8.201(1)
<i>c</i> [Å]	7.523(6)	7.498
α [°]	90	90
β [°]	124.37(5)	124.25(1)
γ [°]	90	90
<i>V</i> [Å ³]	485.28	485.051
<i>Z</i>	4	4
ρ_{calc} [g cm ⁻³]	1.684	1.685
<i>T</i> [K]	295	295

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Urotropinium dinitrate

Name [German, acronym]: Urotropine dinitrate [UDN]
Main (potential) use: Improvised explosive, HMX precursor
Structural formula:



	UDN	
Formula	C ₆ H ₁₄ N ₆ O ₆	
Molecular mass [g mol ⁻¹]	265.21	
Appearance at RT		
IS [J]	15 (<100 μm)	
FS [N]	240 (<100 μm)	
ESD [J]	1.3 (<100 μm)	
N [%]	31.57	
Ω(CO ₂) [%]	-78.43	
T _{m,p.} [°C]	160	
T _{dec.} [°C]	164 (DSC @ 5 °C/min)	
ρ [g cm ⁻³]	1.711 (@ 173 K), 1.663 (@ 298 K, gas pycnometer)	
Heat of formation	-470 kJ/mol (Δ _f H°), -1,645 kJ/kg (Δ _f U°)	
	Calcd. (EXPLO5 6.03)	Exptl.
-Δ _{ex} U° [kJ kg ⁻¹]	3,222	
T _{ex} [K]	2,239	
p _{C-J} [kbar]	210	
VoD [m s ⁻¹]	7,726	
V ₀ [L kg ⁻¹]	860	

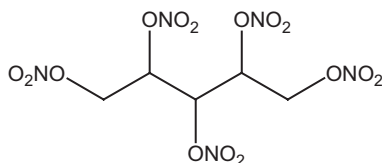
X

Xylitol pentanitrate

Name [German, acronym]: 1,2,3,4,5-Pentakis-nitrooxy-pentane [XPN]

Main (potential) use: Previously proposed as possible candidate for use in solid rocket propellant formulations, but later shown to be a sensitive primary explosive^[2]

Structural formula:



	XPN
Formula	C ₅ H ₇ N ₅ O ₁₅
Molecular mass [g mol ⁻¹]	377.13
Appearance at room temperature	Colorless solid ^[1] , white crystalline solid ^[2]
IS [J]	Detonated under hammer ^[1] , Fol = 25 (average gas evolution = 6 mL, Rotter impact analysis, cf. RDX Fol = 80) ^[2]
FS [N]	18 (faint cracking sound, 10 mg sample, Julius-Peters apparatus, BAM) ^[2]
ESD [J]	4.5 but not at 0.45 (DSTO apparatus) ^[2]
N [%]	18.57
Ω(CO ₂) [%]	6.36
T _{m.p.} [°C]	37–40 ^[1] , 45.5 (DSC @ 10 °C/min) ^[2] , 40 ^[4]
T _{dec.} [°C]	169.5 (exo, onset) 185.8 (exp, peak max) (DSC @ 10 °C/min) ^[2] , 174.8 (exo, onset), 184.8 (exo, peak max) (DSC @ 10 K/min) ^[4, 5]

Thermal stability	No dec. observed after storing for 3 years @ 0–5 °C in desiccator ^[1] , critical <i>T</i> for thermal dec. = 140.1 °C ^[4]
Solubility [g/mL]	Recryst. from toluene ^[1] , recryst. from EtOH/H ₂ O ^[2]
Compatibility	Dec. in pyridine ^[1]
ΔH_{dec} [J/g]	353 (DSC @ 10 °C/min) ^[2] , 208.9 kJ/mol ^[4] , 661.0 (DSC @ 10 K/min) ^[5]
Heat capacity, $C_{p,m}$ [J•mol ^{−1}]	273.24 @ 200 °C (calcd.) ^[3] , 358.85 @ 298,15 °C (calcd.) ^[3] , 360.39 @ 300 °C (calcd.) ^[3] , 436.72 @ 400 °C (calcd.) ^[3] , 498.15 @ 500 °C (calcd.) ^[3] , 546.10 @ 600 °C (calcd.) ^[3] , 583.56 @ 700 °C (calcd.) ^[3] , 613.19 @ 800 °C (calcd.) ^[3]
Activation energy to thermal dec. [kJ/mol]	159 (liquid, SMM) ^[4] , 140 ± 1.9 (@ 131–213 °C, TG) ^[4, 5] , 146.9 kJ/mol ^[5]

	XPN ^[2]
Chemical formula	C ₅ H ₇ N ₅ O ₁₀
Molecular weight [g mol ^{−1}]	377.16
Crystal system	Monoclinic
Space group	<i>P</i> 2 ₁ / <i>c</i>
<i>a</i> [Å]	8.0945(3)
<i>b</i> [Å]	15.9392(6)
<i>c</i> [Å]	10.4903(5)
α [°]	90
β [°]	91.684(3)
γ [°]	90
<i>V</i> [Å ³]	1,352.87(10)
<i>Z</i>	4
ρ_{calc} [g cm ^{−3}]	1.852
<i>T</i> [K]	150
	Recryst. from EtOH/H ₂ O by slow evaporation

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