Thomas M. Klapötke

Energetic Materials Encyclopedia

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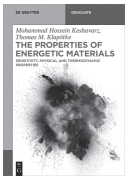

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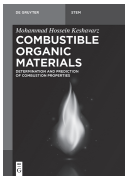

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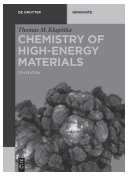

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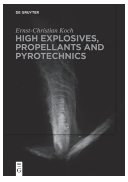

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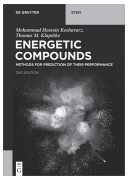

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Thomas M. Klapötke

Energetic Materials Encyclopedia

E–N

DE GRUYTER

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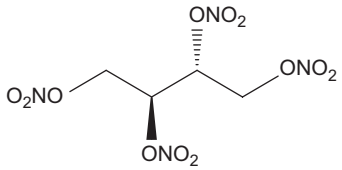
E

Erythritol tetranitrate

Name [German, acronym]: Erythritol tetranitrate, butane-1,2,3,4-tetrayl tetranitrate, meso-erythritol tetranitrate, erythritetetranitrate, tetranitroerythrite, nitro-*i*-erythrite, 1,2,3,4-butanetetrol tetranitrate, nitroerythrite, erythrol tetranitrate, tetranitrol, tetranitrin, nitroerythrite, cardilate, cardiloid [ETN, ErTN, ErTeN]

Main (potential) use: Improvised explosive, suggested as an addition to smokeless powders[13], melt-castable explosive[17]

Structural formula:



	ETN
Formula	$C_4H_6N_4O_{12}$
Molecular mass [g mol^{-1}]	302.11
Appearance at room temperature (RT)	Colorless plates, white solid[13, 14], leaflets (from EtOH)[21, 22]
IS [J]	3 (100–500 µm), 24.0 cm with 4 kg mass (LLNL-apparatus, Bruceton method)[2], 20 cm (2 kg mass, B.M.)[5], 3.28 (impact energy for 50% probability of initiation, Kast apparatus, crystalline ETN)[9], 3.79 (impact energy for 50% probability of initiation, Kast apparatus, melt-cast ETN)[9], similar to NG[14], DH_{50} = 24.0 cm (4 kg mass, Bruceton method, 35 mg sample, 120 grit sandpaper, LLNL small-scale apparatus)[2], H_{50} = 38 cm (design no. 3 apparatus)[24], H_{50} = 4.6 cm (design no. 12 apparatus, 6 units cf. TNT = 100 units)[24] DH_{50} (ERL apparatus, type 12 tool, 2.5 kg mass, 150 grit paper): 6.4 ± 2 cm (crystals from MeOH)[7], 6.3 ± 2 cm (small crystals from acetone/EtOH)[7], 6.2 ± 2 cm (solid precipitate)[7], 6.4 ± 2 cm (crystal sheets)[7]

https://doi.org/10.1515/9783110672565-005

<table>
<tr><td>FS [N]</td><td>60 (100–500 µm), 38.9 (friction force for 50% probability of initiation, crystalline ETN)[9], 47.7 (friction force for 50% probability of initiation, melt-cast ETN)[9]
F_{50} (BAM apparatus, 2–5 mg samples): 57 ± 11 (crystals from MeOH)[7], 52 ± 15 (small crystals from acetone)[7], 54 ± 15 (solid precipitate)[7], 48 ± 11 (crystal sheets)[7], 67 ± 7 (crash precipitate)[7]</td></tr>
<tr><td>ESD [J]</td><td>0.15

Threshold initiation level (SMS ABL apparatus): 0.0625 (crystals from MeOH)[7], 0.0625 (small crystals from acetone/EtOH)[7], 0.0625 (solid precipitate)[7], 0.125 (crystal sheets)[7], 0.0625 (crash precipitate)[7]</td></tr>
<tr><td>N [%]</td><td>18.55</td></tr>
<tr><td>$\Omega(CO_2)$ [%]</td><td>+5.30</td></tr>
<tr><td>$T_{m.p.}$ [°C]</td><td>61[5, 13, 14, 16, 21, 22], 63.5 (melt) (DSC @ 10 °C/min, under N_2 flow, crystals slowly grown from CH_3OH)[7], 61.5 (melt) (DSC @ 10 °C/min, under N_2 flow, solid precipitate from CH_3CN/H_2O)[7], 58.7 (onset), 60.5 (endo) (DSC @ 10 °C/min)[12], 61.2 (onset), 63.7 (peak max), 66.0 (end T) (DSC @ 10.0 K/min, pinhole cover)[15], 58–59 (crude from mixed nitration)[2], 60–61 (recryst.)[2], 59.6–61.0 (crude ETN from nitration with acetyl nitrate)[2], 60.5–61.0 (recryst. from 2-propanol)[2]

DSC, flame sealed in glass microampules, N_2, @ 50 mL/min[2]:
<table>
<tr><th>Heating rate (K/min)</th><th>n</th><th>Mass (mg)</th><th>Endotherm, T_{min} (°C)</th><th>ΔH_{fus} (J/g)</th></tr>
<tr><td>20</td><td>4</td><td>0.203</td><td>60</td><td>113</td></tr>
<tr><td>10</td><td>5</td><td>0.200</td><td>62</td><td>107</td></tr>
<tr><td>9</td><td>6</td><td>0.288</td><td>63</td><td>105</td></tr>
<tr><td>8</td><td>5</td><td>0.244</td><td>63</td><td>102</td></tr>
<tr><td>7</td><td>4</td><td>0.255</td><td>61</td><td>117</td></tr>
<tr><td>6</td><td>1</td><td>0.232</td><td>63</td><td>102</td></tr>
<tr><td>5</td><td>2</td><td>0.226</td><td>59</td><td>116</td></tr>
<tr><td>4</td><td>2</td><td>0.219</td><td>62</td><td>104</td></tr>
<tr><td>3</td><td>3</td><td>0.255</td><td>60</td><td>114</td></tr>
<tr><td>2</td><td>2</td><td>0.281</td><td>61</td><td>99</td></tr>
<tr><td>1</td><td>6</td><td>0.292</td><td>59</td><td>109</td></tr>
</table>
61.2 (endo, onset), 63.7 (endo, peak max.) (DSC 10 K/min)[25]</td></tr>
</table>

$T_{dec.}$ [°C]

162.5 (onset), 200.2 (peak max.) (DSC @ 10 °C/min, under N_2 flow, crystals slowly grown from CH_3OH)[7], 164.2 (onset), 198.4 (peak max.) (DSC @ 10 °C/min, under N_2 flow, solid precipitate from CH_3CN/H_2O)[7], 192.6 (DSC @ 10 °C/min)[12], 184.8 (onset), 196.3 (peak max), 211.6 (end *T*) (DSC @ 10.0 K/min, pinhole cover)[15], 200 (DTA, max mass loss @ 10 K/min, 8–10 mg sample, open Pt pan)[2]

DSC, flame sealed in glass microampules, N_2, @ 50 mL/min[2]:

Heating rate (K/min)	*n*	Mass (mg)	Exotherm, T_{min} (°C)	Exotherm, T_{max} (°C)	Δ*H* (J/g)
20	4	0.203	184	199	2,233
10	5	0.200	182	193	2,795
9	6	0.288	183	192	2,592
8	5	0.244	182	191	2,437
7	4	0.255	182	186	3,181
6	1	0.232	181	185	2,418
5	2	0.226	176	180	3,253
4	2	0.219	176	180	2,948
3	3	0.255	171	173	2,957
2	2	0.281	168	169	2,551
1	6	0.292	155	156	3,130

Nonisothermal TG data[25]:

β (K min^{-1})	T_{ot}	T_i	Mass loss (%)		L_{max} (% min^{-1})	T_p (°C)	T_{oe} (°C)
			Stage 1	Residue (%)			
5.0	157.1	98.6	97.60	0.64	–21.65	174.6	184.1
7.0	160.5	99.3	99.67	0.22	–28.03	177.6	192.4
10.0	165.4	100.2	99.46	0.09	–39.95	183.1	196.3
15.0	169.3	101.2	99.87	0.43	–59.63	186.2	202.8

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

184.8 (exo, onset), 196.3 (exo, peak max) (DSC 10 K/min)[25]

ρ [g cm^{-3}]

1.840 (@ 100 K), 1.759 (@ 291 K), 1.774 (@ 298 K, gas pycnometer), 1.851 (crystal @ 140 K)[7], 1.50 (loading ρ)[5], 1.773 (@ TMD)[17], 1.7219 (pycnometer)[2], 1.55 (X-ray)[2]

Heat of formation	376 cal/g (@ C^V)[5], −474.8 kJ/mol ($\Delta_f H$)[2, 16], 369.2 kcal/kg (Q)[18], 130.5 cal (molecular heat of formation)[22], −114.76 kcal/mol ($\Delta H_f°$)[23]		
Heat of combustion	1,546 cal/g (@ C^V)[5, 18], 2,790.9 kJ/mol (ΔH_c, heat of comb.)[25]		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]	6,105	10.11 kJ cm^{-3} (@ 1.773 g cm^{-3}, 96% TMD, total energy of det., ΔH_f = 376 cal/g, calcd., CHEETAH 6.0, JWL)[17] 154.7 kcal/100 g (@ 1.50 g cm^{-3}, constant volume) [H_2O (l)][19] 1414 cal/kg (heat of explosion @ constant volume, H_2O (g))[22]	6,025 [H_2O (g)][3] Q_e^P = 1,467.7 kcal/kg[6] Q_e^V = 1,486.0 kcal/kg[6]
T_{ex} [K]	4,225	4,565[5] 4,565 °C (@ 1.50 g cm^{-3})[19]	T_e^P = 4,729.8 °C[6] T_e^V = 4,759.0 °C[6]
$p_{C\text{-}J}$ [kbar]	301	26.77 GPa (@ 1.7219 g cm^{-3} (pycnometry density), heat of formation = −474.8 kJ/mol, Cheetah 6.0)[2] 3.274 GPa (@ 0.69 g cm^{-3} (small-scale explosivity device (SSED) density), heat of formation = −474.8 kJ/mol, Cheetah 6.0)[2]	

VoD [m s^{-1}]	8,540	8,300 (@ 1.760 g cm^{-3}, calcd. K-J)[15] 8,113 (@ 1.773 g cm^{-3}, 96% TMD, ΔH_f = 376 cal/g, calcd., CHEETAH 6.0)[17] 8,206 (@ 1.7219 g cm^{-3} (pycnometry density), heat of formation = –474.8 kJ/mol, CHEETAH 6.0)[2] 3,998 (@ 0.69 g cm^{-3} (SSED density), heat of formation = –474.8 kJ/mol, CHEETAH 6.0)[2]	8,100 (@ 1.6 g cm^{-3})[4] 4,240 (@ 0.83 g cm^{-3}, hand-pressed, crystalline powder, ionization probes and digital oscilloscope)[9] 4,630 (@ 0.86 g cm^{-3})[9] 7,940 (@ 1.65 g cm^{-3}, melt cast)[9] 8,030 (@ 1.70 g cm^{-3}, melt cast)[9] 8.03 ± 0.04 mm μs^{-1} (@ 1.74 g ± 0.01 cm^{-3}, 98% TMD, small scale, unconfined detonation rate stick @ 6.35 ± 0.03 mm pellet diameter)[17] 7.97 ± 0.02 mm μs^{-1} (@ 96% TMD, average exptl. value)[17] 7.887 ± 0.007 mm μs^{-1} (@ 1.682 g ± 0.019 cm^{-3}, 94.9% TMD, Cu 0.5 in cylinder test)[17] 7.994 ± 0.022 mm μs^{-1} (@ 1.704 g ± 0.010 cm^{-3}, 96.1% TMD, Cu 0.5 in cylinder test)[17] 7.90 ± 0.13 mm μs^{-1} (@ 1.74 g ± 0.01 cm^{-3}, 98% TMD, small scale, unconfined detonation rate stick @ 3.00 ± 0.03 mm pellet diameter)[17]

V_0 [L kg^{-1}]	767	70.5 L/100 g (@ 1.50 g cm^{-3}, @ STP)	704 (@ 1.7 g cm^{-3})[1] 704.8[6] 705[8, 15]
I_{sp} [Ns g^{-1}]	2.34 (calcd., ISPBKW code)[23], 2.43 (calcd., empirical)[23]		

Critical diameter [cm]	<3 mm (small scale, unconfined detonation rate sticks)[17]
Critical *T* for thermal dec. [°C]	162.5 (TG)[15], critical *T* for thermal dec. = 162.6 °C[25]
Trauzl test [cm^3, % TNT]	550 cc (10 g sample, cf. 285 cc for TNT)[5], 550[20]
Sand test [g]	132–143% TNT[10]
Ballistic mortar test	151% TNT[10]
5 s explosion *T* [°C] Explosion *T* [°C]	220 (205)[5] 275/0.108 s (3 mg sample)[11], 239/0.475 s (3 mg sample)[11], 205/4.95 s (3 mg sample)[11], 200/no action (3 mg sample)[11]
Thermal stability	Nonisothermal TG data, β = °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.[15]:

β (°C/min)	T_{ei} (°C)	T_p (°C)	T_{oe} (°C)	T_b (°C)
5.0	157.1	174.6	184.1	162.5
7.0	160.5	177.6	192.4	
10.0	165.4	183.1	196.3	
15.0	169.3	186.2	202.8	

Vapor pressure [atm. @ °C]	3.19 × 10^{-3} Pa @ 25 °C[2]
Burn rate [mm/s]	Should not be burned as even small amount of confinement of a small sample can result in a violent explosion[17]
Solubility [g/mL]	Can be recrystallized from EtOH[13], soluble in EtOH[17], soluble in MeOH, EtOH, 2-propanol, acetone and acetonitrile[2], soluble in EtOH, Et_2O, glycerol[21], insoluble in water[21], insoluble in cold water[22]
$\Delta H_{melting}$ [J/g]	–297.7 (heat absorption, DSC @ 10 K/min, pinhole cover)[15]
ΔH_{dec} [J/g]	364.3 (heat release, DSC @ 10 K/min, pinhole cover)[15], 137.4 kJ/mol (ΔH_d, heat of dec.)[25]
ΔH_{sub} [J/g]	117.7[2]

SSED	British.303 cartridge, 2 g explosive, RP-3 EBW[2]:

Charge depth (mm)	Tap density (g mL^{-1})	Mass cartridge (g)	Mass remaining (g)	Fraction remaining (%)
18	0.71	11.027	3.0412	27.6
25	0.91	10.9242	3.0325	27.8
9	0.58	11.1935	3.1628	28.3
14	0.64	11.2962	2.994	26.5
29	1.07	10.987	3.3665	30.6
30	1.07	11.2383	3.1386	27.9

	Erythritol tetranitrate[7]	**Erythritol tetranitrate**[7]	**Erythritol tetranitrate**[8]
Chemical formula	$C_4H_6N_4O_{12}$	$C_4H_6N_4O_{12}$	$C_4H_6N_4O_{12}$
Molecular weight [g mol^{-1}]	302.13	302.13	302.13
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	$P\,2_1/c$ (no. 14)	$P\,2_1/c$ (no. 14)	$P\,2_1/c$ (no.14)
a [Å]	16.132(6)	15.893(6)	15.9681(10)
b [Å]	5.314(2)	5.1595(19)	5.1940(4)
c [Å]	14.789(6)	14.731(5)	14.7609(12)
α [°]	90	90	90
β [°]	116.78(4)	116.161(3)	116.238(6)
γ [°]	90	90	90
V [$Å^3$]	1,132(1)	1,084.2(7)	1,098.10(15)
Z		4	4
ρ_{calc} [g cm^{-3}]	1.773	1.851	1.827
T [K]	RT	140	–123 °C

ETN crystallizes out of EtOH as leaflets[22]

[1] M. Jafari, M. Kamalvand, M. H. Keshavarz, A. Zamani, H. Fazeli, *Indian J. Engineering and Mater. Sci.*, **2015**, *22*, 701–706.

[2] J. C. Oxley, J. L Smith, J. E. Brady, A. C. Brown, *Propellants, Explosives and Pyrotechnics*, **2012**, *37*, 24–39.

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[4] P. W. Cooper, *Explosives Engineering*, Wiley-VCH, New York, **1996**.

[5] B. T. Fedoroff, O. E. Sheffield, *Encyclopedia of Explosives and Related Items*, *vol. 5*, US Army Research and Development Command, TACOM, Picatinny Arsenal, USA, **1972**.
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[10] 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**.
[11] B. T. Fedoroff, O. E. Sheffield, *Encyclopedia of Explosives and Related Items*, *vol. 6*, US Army Research and Development Command, TACOM, Picatinny Arsenal, USA, **1974**.
[12] J. C. Oxley, D. Furman, A. C. Brown, F. Dubnikova, J. L. Smith, R. Kosloff, Y. Zeiri, *J. Phys. Chem. C*, **2017**, *121*, 16145–16157.
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[17] V. W. Manner, D. N. Preston, B. C. Tappan, V. E. Sanders, G. W. Brown, E. Hartline, B. Jensen, *Propellants, Explosives, Pyrotechnics*, **2015**, *40*, 460–462.
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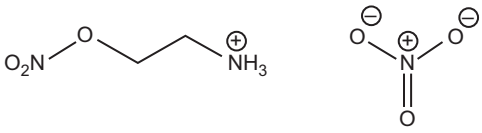
Ethanolamine dinitrate

Name [German, acronym]: Ethanolamine dinitrate, 2-nitratoethylammonium nitrate, ethanolamine nitric ester nitrate [monoethanolamindinitrat]

Main (potential) use:

Structural formula:



	Ethanolamine dinitrate	
Formula	$C_2H_7N_3O_6$	
Molecular mass [g mol^{-1}]	169.09	
Appearance at RT	Solid[3]	
N [%]	24.85	
Ω(CO_2) [%]	−14.2	
$T_{m.p.}$ [°C]	103[1, 3]	
ρ [g cm^{-3}]	1.53[1]	
Heat of formation		
	Calcd. (EXPLO5 6.04)	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]		5,247 [H_2O (l)][1] 4,557 [H_2O (g)][1]
T_{ex} [K]		
$p_{C\text{-}J}$ [GPa]		
VoD [m s^{-1}]		
V_0 [L kg^{-1}]		927[1, 2]

Trauzl test [cm^3, % TNT]	430 cm^3[3]

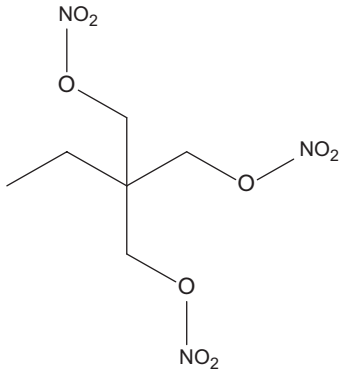
[1] R. Meyer, J. Köhler, A. Homburg, *Explosives*, 7th edn., Wiley-VCH, Weinheim, **2016**, p. 125.
[2] M. Jafari, M. Kamalvand, M. H. Keshavarz, A. Zamani, H. Fazeli, *Indian J. Engineering and Mater. Sci.,* **2015**, *22,* 701–706.
[3] T. Urbański, Ch. 19 in *Chemistry and Technology of Explosives*, *vol. II*, **1965**, Pergamon Press, Oxford.

Ethriol trinitrate

Name [German, acronym]: 2-Ethyl-2-(hydroxymethyl)-1,3-propanedioltrinitrate, trimethylolpropane trinitrate [TMPTN]

Main (potential) use: propellant charge

Structural formula:



	Ethriol trinitrate
Formula	$C_6H_{11}N_3O_9$
Molecular mass [g mol^{-1}]	269.17
Appearance at RT	Solid[6], colorless crystals[3]
N [%]	15.61
Ω(CO_2) [%]	−50.5
$T_{m.p.}$ [°C]	50.3[1], 51[3], 50.3 (onset), 53.6 (peak max.), 58.4 (end *T*) (DSC @ 10.0 K/min, pinhole cover)[5], 50.3 (endo, onset), 53.6 (endo, peak max.) (DSC 10 K/min)[7]
$T_{dec.}$ [°C]	181.9[1], 181.9 (onset), 206.4 (peak max.), 221.8 (end *T*) (DSC @ 10.0 K/min, pinhole cover)[5], 181.9 (exo, onset), 206.4 (exo, peak max.) (DSC 10 K/min)[7]

<table>
<tr><td></td><td>Nonisothermal TG data[7]:

<table>
<tr><th rowspan="2">β (K min^{-1})</th><th rowspan="2">T_{ot}</th><th rowspan="2">T_i</th><th colspan="2">Mass loss (%)</th><th rowspan="2">$L_{max.}$ (% min^{-1})</th><th rowspan="2">T_p (°C)</th><th rowspan="2">T_{oe} (°C)</th></tr>
<tr><th>Stage 1</th><th>Residue (%)</th></tr>
<tr><td>5.0</td><td>159.7</td><td>95.7</td><td>99.05</td><td>0.56</td><td>–20.71</td><td>178.8</td><td>186.6</td></tr>
<tr><td>7.0</td><td>167.1</td><td>96.3</td><td>98.24</td><td>1.84</td><td>–27.48</td><td>185.7</td><td>197.8</td></tr>
<tr><td>10.0</td><td>170.7</td><td>97.2</td><td>99.15</td><td>0.12</td><td>–37.42</td><td>191.0</td><td>203.4</td></tr>
<tr><td>15.0</td><td>180.5</td><td>98.5</td><td>98.99</td><td>0.18</td><td>–62.25</td><td>196.8</td><td>211.6</td></tr>
</table>

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</td></tr>
<tr><td>ρ [g cm^{-3}]</td><td>1.454 ± 0.06 (@ 293.15 K)[2], 1.5[3]</td></tr>
<tr><td>Heat of formation</td><td>–426 kcal/kg (enthalpy of form.)[3], –1,783 kJ/kg (enthalpy of form.)[3], –479.9 kJ/mol (enthalpy of form., exptl.)[6], –451.2 kJ/mol (enthalpy of form., calcd., emp.)[6], –461.6 kJ/mol (enthalpy of form., calcd., S-D method)[6]</td></tr>
<tr><td>Heat of combustion</td><td>2,175.5 kJ/mol (ΔH_c, heat of comb.)[7]</td></tr>
<tr><td></td><td></td></tr>
<tr><td></td><td>Calcd. (EXPLO5 6.04)</td><td>Lit. values</td><td>Exptl.</td></tr>
<tr><td></td><td></td><td></td><td></td></tr>
<tr><td>$-\Delta_{ex}U^{o}$ [kJ kg^{-1}]</td><td>4,834</td><td>1,449.9 (calcd., K-J)[4]</td><td>4,244 [H_2O (l)][3]

3,916 [H_2O (g)][3]</td></tr>
<tr><td>T_{ex} [K]</td><td>3,237</td><td></td><td></td></tr>
<tr><td>$p_{C\text{-}J}$ [Gpa]</td><td>19.6</td><td>26.65 (calcd., K-J)[4]</td><td></td></tr>
<tr><td>VoD [m s^{-1}]</td><td>7,097 (@ 1.5 g cm^{-3}; $\Delta_f H$ = –480 kJ mol^{-1})</td><td>7,490 (@ 1.5 g cm^{-3}, calcd., K-J)[1]</td><td>6,440 (@ 1.48 g cm^{-3}, confined)[3]</td></tr>
<tr><td>V_0 [L kg^{-1}]</td><td>804</td><td></td><td>1,009[3]</td></tr>
</table>

<table>
<tr><td></td><td></td></tr>
<tr><td>Thermal stability</td><td>Nonisothermal TG data, β = °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.[5]:

<table>
<tr><td>β (°C/min)</td><td>T_{ei} (°C)</td><td>T_p (°C)</td><td>T_{oe} (°C)</td><td>T_b (°C)</td></tr>
<tr><td>5.0</td><td>159.7</td><td>178.8</td><td>186.6</td><td>119.1</td></tr>
<tr><td>7.0</td><td>167.1</td><td>185.7</td><td>197.8</td><td></td></tr>
<tr><td>10.0</td><td>170.7</td><td>191.0</td><td>203.4</td><td></td></tr>
<tr><td>15.0</td><td>180.5</td><td>196.8</td><td>211.6</td><td></td></tr>
</table>
Critical T for thermal dec. = 169.3 °C[7]</td></tr>
<tr><td>ΔH_{melt} [J/g]</td><td>–114.8 (heat absorption)[5]</td></tr>
<tr><td>$\Delta H_{dec.}$ [J/g]</td><td>1,105 (heat release)[5], 499.7 kJ/mol (ΔH_d, heat of dec.)[7]</td></tr>
</table>

[1] Q.-L. Yan, M. Künzel, S. Zeman, R. Svoboda, M. Bartoskova, *Thermochimica Acta*, **2013**, *566*, 137–148.

[2] Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© **1994–2017** ACD/Labs).

[3] R. Meyer, J. Köhler, A. Homburg, *Explosives*, 7th edn., Wiley-VCH, Weinheim, **2016**, p. 126.

[4] M.-M. Li, G.-X. Wang, X.-D. Guo, Z.-W. Wu, H.-C. Song, *Journal of Molecular Structure: THEOCHEM,* **2009**, *900*, 90–95.

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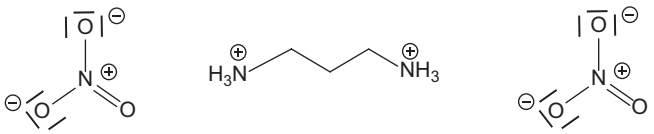
Ethylenediamine dinitrate

Name [German, acronym]: Ethylenediamine dinitrate, ethylenediammonium dinitrate, diamin [PH-Salz, EDD, EDAD, EDDN]

Main (potential) use: Used as ingredient of fusible mixtures containing AN (PH-Salz) in World War II[14], was used as a bursting charge[10, 17], phlegmatized EDD was used as bursting charge in anticoncrete shells[18], was used as cast charge in eutectic mixtures with AN[10], mixtures with wax used in boosters in World War II[10]

Structural formula:



	EDD
Formula	$C_2H_{10}N_4O_6$
Molecular mass [g mol^{-1}]	186.12
Appearance at RT	White crystals[10], crystalline solid, colorless when pure[17]
IS [J]	10 Nm[1], 75 cm (B.M.)[10], 9 in (P.A.)[10], FI = 120% PA[11], $H_{50\%}$ = 2.50 m (10 kg mass, mouton, French test)[11], $H_{50\%}$ = 34.2 cm (2.5 kg mass, B.M. model 2, 35 mg sample, 80–325 mesh, 180 grit paper, Bruceton test)[13], $H_{50\%}$ = 18.0 cm (5.0 kg mass, B.M. model 2, 35 mg sample, 80–325 mesh, 180 grit paper, Bruceton test)[13]
FS [N]	>353[1]
ESD [J]	$E_{50\%}$ = 0.64 ± 0.06 (Bruceton method)[15]
N [%]	30.10
Ω(CO_2) [%]	−25.8
$T_{m.p.}$ [°C]	188.6[2], 185–187[10, 11, 17], 188.1[13], 185[18]
$T_{dec.}$ [°C]	275[3], 270 (dec. with liberation of brown fumes)[17]
ρ [g cm^{-3}]	1.577[1], sp. gr. = 1.595 (@ 25/40)[10], 1.595[4, 13], 1.603 (pycnometry)[13], sp. gr. = 1.595 (@ 25/4°)[11], 1.49 (pelleted under a pressure of 1,500 kg cm^2, Kast)[14]
Heat of formation	−653.5 kJ/mol[4], 156.1 kcal/mol[10, 11], −3,511.2 kJ/kg[4], −839.2 kcal/kg (enthalpy of form.)[1, 9], 803.6 kcal/kg (*Q*)[19], −839.0 kcal/kg (enthalpy of form.)[16], 117.29 kcal/mol (−ΔH_f (heat of form. @ standard conditions))[21]

<table>
<tr><td>Heat of combustion</td><td colspan="3">−374.7 kcal/mol[11], 374.7 kcal/mol (@ C^p)[10], 2,020 kcal/kg (@ C^v)[19]

Exptl. heat of combustion data[21]:<table><tr><th>$-\Delta U_{B/M}$ (cal/g)</th><th>$-\Delta U_B$ (kcal/mol)</th><th>$-\Delta U_R$ (kcal/mol @ 1 atm. and constant vol.)</th><th>$-\Delta H_R$ (kcal/ mol @ 1 atm. and constant pressure)</th></tr><tr><td>2,016.26 ± 0.79</td><td>375.29</td><td>374.70</td><td>373.22</td></tr></table></td></tr>
<tr><td></td><td colspan="3"></td></tr>
<tr><td></td><td>Calcd. (EXPLO5 6.04)</td><td>Lit. values</td><td>Exptl.</td></tr>
<tr><td></td><td></td><td></td><td></td></tr>
<tr><td>$-\Delta_{ex}U^{\circ}$ [kJ kg^{-1}]</td><td></td><td>3,447 (calcd., K-J)[5]

931 kcal/kg (@ 1.550 g cm^{-3}, calcd.) [H_2O vapor][16]</td><td>3,814 [H_2O (l)][1, 5]

3,091 [H_2O (g)][1]

890 kcal/kg [H_2O (g)][9]

127.9–159.3 kcal/mol[10, 11]

890 kcal/kg (@ 1.550 g cm^{-3}) [H_2O vapor][16]</td></tr>
<tr><td>T_{ex} [K]</td><td></td><td>1,670 (calcd., K-J)[6]</td><td></td></tr>
<tr><td>$p_{C\text{-}J}$ [GPa]</td><td></td><td>24.233 (calcd., K-J)[4]</td><td></td></tr>
<tr><td>VoD [m s^{-1}]</td><td></td><td>7,930 (@ 1.55 g cm^{-3}, calcd., K-J)[6]

8,090 (@ 1.60 g cm^{-3} (TMD))[12]</td><td>VoD can reach 6,800 (30 diameter cardboard tube)[14]

6,800 (@ 1.53 g cm^{-3}, confined)[1]

7,550[6]

7,690 (@ 1.60 g cm^{-3})[7]

4,650 (@ sp. gr. = 1.0, Dautrische method)[10, 11]

6,270 (@ sp. gr. = 1.33, Dautrische method)[10, 11]

6,915 (@ sp. gr. = 1.50, Dautrische method)[10, 11]</td></tr>
<tr><td>V_0 [L kg^{-1}]</td><td></td><td></td><td>1,071[1, 8]</td></tr>
</table>

Trauzl test [cm^3, % TNT]	120–125% TNT[10], 125% TNT[10, 11], 115% PA[11], 345 cm^3[14], 350[20]
Sand test [g]	96% TNT[10]
Ballistic mortar test	114% TNT[11]
Ballistic pendulum test	114% TNT[10]
Initiation efficiency	0.10 g tetryl minimum detonating charge (sand test)[10], 2 g MF required for initiation of 50 g sample of sp. gr. = 1.23 in paper cylinder with 30 mm diameter[10]
Gap test	3.75 cm between paper cartridges each containing 50 g sample (@ 0.75 g cm^{-3})[10, 11]
5 s explosion *T* [°C] 1 s ignition test [°C] 6 s ignition *T* [°C] Explosion *T* test [°C]	 430[10, 11] 370[10, 11] 445[10]
Thermal stability	Vaporizes and condenses without dec. when heated in vacuum[10], autocatalytic dec. on heating between 230–360 °C under 100 mm pressure in nitrogen atmosphere[10], 0.38% weight loss after 14 days @ 75 °C[14], no explosion on heating up to 350 °C[14]
Vacuum stability test [cm^3/h]	5 mL gas evolved @ 120 °C[10]
Burn rate [mm/s]	Ignited by open flame after 60 s and continues burning at rate of 1.5 cm/min[10]
Solubility [g/mL]	Soluble in water but insoluble in Et_2O or EtOH[10], eutectic formed with AN[10], immiscible with molten TNT[10], readily soluble in H_2O[17]
Hygroscopicity	1.24% @ 25 °C and 90% RH[10], hygroscopic[14]
Rifle bullet impact test	No detonations with bullet velocities >960 m/s (sp. gr. of charge = 1.0)[10], incomplete detonations with bullet velocities ~1,000 m/s (sp. gr. of charge = 1.0)[10]
Plate dent test	Essentially identical with the values of TNT[10]

[1] R. Meyer, J. Köhler, A. Homburg, *Explosives*, 7th edn., Wiley-VCH, Weinheim, **2016**, pp. 126–127.
[2] Y.-H. Kong, Z.-R. Liu, Y.-H. Shao, C.-M. Yin, W. He, *Thermochimica Acta*, **1997**, *297*, 161–168.
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[6] T.-Z. Wang, G.-G. Xu, J.-P. Xu, Y.-J. Liu, *Journal Beijing Institute of Technology* **2000**, *9*, 341–346.
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[8] M. Jafari, M. Kamalvand, M. H. Keshavarz, A. Zamani, H. Fazeli, *Indian J. Engineering and Mater. Sci.*, **2015**, *22*, 701–706.
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[10] *Military Explosives*, Department of the Army Technical Manual, TM 9-1300-214, Headquarters, Department of the Army, September **1984**.
[11] B. T. Fedoroff, O. E. Sheffield, *Encyclopedia of Explosives and Related Items*, *vol. 6*, US Army Research and Development Command, TACOM, Picatinny Arsenal, USA, **1974**.
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[13] R. L. McKenney, S. R. Struck, R. A. Hildreth, J. A. Fryling, *J. Energet. Mater.*, **1987**, *5*, 1–25.
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[17] *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**.
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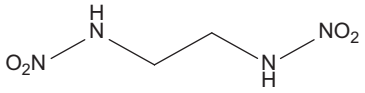
[19] Y. Y. Orlova, *The Chemistry and Technology of High Explosives, Part III*, translated by the Technical Documents Liaison Office, Wright Patterson Air Force Base, Ohio, Technical AD261783, Armed Services Technical Information Agency, Virginia, USA, 23rd June **1961**.
[20] M. Jafari, M. Kamalvand, M. H. Keshavarz, S. Farrashi, *ZAAC*, **2015**, *641*, 2446–2451.
[21] 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**.

Ethylene dinitramine

Name [German, acronym]: 1,4-Dinitro-1,4-diazabutane, ethylenedinitramine, *N*,*N*'-dinitroethanediamine, *s*-bisnitroaminoethane ethylene dinitroamine, *N*,*N*'-dinitroethylene diamine, haleite, halite, 1,2-dinitrodiaminoethane, *N*,*N*'-dinitro-1,1-ethane-diamine [äthylendinitramin, EDNA]

Main (potential) use: Component of ednatol[1, 11], boosters, bursting charge[11]

Structural formula:



	EDNA
Formula	$C_2H_6N_4O_4$
Molecular mass [g mol^{-1}]	150.09
Appearance at RT	White solid[22], white – buff-colored crystalline solid[34], white crystals of rhombic shape[37]
IS [J]	8 Nm[1], 8.33[5, 8, 9], 9.42 (B.M.)[11, 12], 6.98 (P.A.)[11, 12, 13], log $H_{50\%}$ = 1.53[18], $H_{50\%}$ = 34 cm (US-NOL)[19], 14 in (2 kg mass, 17 mg sample, P.A.)[11, 20, 38], 48 cm (20 mg sample, B.M.)[11, 20, 21], $H_{38\%}$ = 1.5 m (5 kg mass, French test)[21], 10 in (2 kg mass, explodes)[29], 36 cm (NOL)[30], H_{50} = 34 cm (2.5 kg mass, type 12 tool)[32], 6.98 (48 cm, 2 kg mass, 20 mg sample, B.M)[13], 14 in (2 kg mass, 17 mg sample, P.A.)[13], 32 cm (B.M.)[38] IS of various crystal habits (2 kg mass, B.M)[13]: first plate = 55 cm, second plate = 55 cm, bipyramid = 71 cm, Bracydome = 66 cm, sphenoid = 46 cm[13] 65 cm (ERL #3, sample in brass cup 0.308 in inside diameter, 0.01 in thick, 7/8 in height, 5 kg mass)[43], 35 cm (ERL #5, sample in cylindrical cavity 1/16 in deep, 0.376 in inside diameter, 5 kg mass)[43], 38 cm (ERL #12, sample on square of Flint paper, $2^1/_2$ kg mass)[43], $H_{50\%}$ = 32 cm (4 kg mass, B.M. design 5)[43], 30 cm (sensitivity to glancing impact, Hercules sliding rod, sandblasted surfaces, 45° slide angle, 10 lb rod, 30 mg sample)[43], H_{50} = 42.7 ± 0.04 cm (type 12, ERL apparatus)[44], H_{50} = 34 cm[47]

<table>
<tr><td></td><td>Design no. 3 apparatus[48]:
<table><tr><th>Drop height (cm)</th><th>Trials</th><th>% explosions</th></tr><tr><td>15</td><td>20</td><td>0</td></tr><tr><td>20</td><td>20</td><td>0</td></tr><tr><td>30</td><td>?</td><td>5</td></tr><tr><td>40</td><td>20</td><td>17</td></tr><tr><td>45</td><td>20</td><td>25</td></tr><tr><td>50</td><td>20</td><td>40</td></tr><tr><td>70</td><td>20</td><td>50</td></tr><tr><td>80</td><td>40</td><td>47</td></tr><tr><td>85</td><td>40</td><td>70</td></tr><tr><td>90</td><td>40</td><td>67</td></tr><tr><td>95</td><td>20</td><td>80</td></tr></table>
H_{50} = 76 cm (design no. 3 apparatus, 5 kg hammer)[48], H_{50} = 30–40 cm (design no. 3 apparatus)[48], H_{50} = 35 cm (design no. 5 apparatus)[48], H_{50} (average) = 121 cm (design no. 9 apparatus, 2.5 kg hammer)[48], H_{50} = 133 cm (sand-blasted surfaces, 2.5 kg hammer, design no. 10 apparatus)[48], H_{50} = 248 cm (sand-blasted surfaces, nonflush, 2.5 kg hammer, design no. 10 apparatus)[48], H_{50} = 33 cm (2.5 kg hammer, design no. 11 apparatus)[48], H_{50} = 31.5 cm (design no. 12 apparatus, 42 units cf. TNT = 100 units)[48]</td></tr>
<tr><td>FS [N]</td><td>47.4[7, 8, 9], unaffected by steel shoe (friction pendulum test)[13, 22, 38], unaffected by fiber shoe (friction pendulum test)[13, 22], $H_{50\%}$ = 22 cm (friction pendulum, 30 mg sample, sandblasted surface, 2 in ball, 5 kg weight, 8° angle of incidence)[43]</td></tr>
<tr><td>N [%]</td><td>37.33</td></tr>
<tr><td>$\Omega(CO_2)$ [%]</td><td>–32.0</td></tr>
<tr><td>$T_{m.p.}$ [°C]</td><td>180[2], dec. >175[13], 174–178 (dec.)[20, 34], 177.30 (dec.)[11, 22], 177–179 (dec. starts @ 175)[21], 174–176[29], 175–176[37], 176.2 (dec., Mettle mpt. apparatus, @ 1 K/min beginning at 10 K beneath the mpt.)[41]</td></tr>
<tr><td>$T_{dec.}$ [°C]</td><td>186 (DSC @ 5 °C/min)[2], 175+[13], 175 (starts)[21], 174–176[29]</td></tr>
</table>

ρ [g cm^{-3}]	1.65 (@ 298.15 K)[2], 1.749[6], 1.71 (@ TMD)[13], 1.75 (@ 20 °C)[20] 1.55–1.77 (crystal, depending on solvent used for recryst.)[22], sp. gr. = 1.71 (crystal)[21], 1.71 (crystal)[13, 38], sp. gr. = 1.75[37]

ρ (g cm^{-3})	Pressure (psi)
1.28[13, 21, 22]	5,000
1.38[13, 22], 1.39[21]	10,000
1.41[13, 21, 22]	12,000
1.44[13, 21, 22]	15,000
1.49[13, 21, 22]	20,000
1.56[21]	40,000
Loading ρ (g cm^{-3})	Pressure (kpsi)
1.39[23, 38]	5
1.46[23, 38]	10
1.51[23, 38]	15
1.55[23, 38]	20
1.72[23]	(crystal)

Heat of formation	−103.8 kJ/mol ($\Delta_f H^o$)[3], 134 cal/g[13, 19], −691.6 kJ/kg (enthalpy of form.)[1, 3], −661.1 kJ/kg[6], −169.0 kcal/kg ($\Delta_f H$)[17], 20.11 kg cal/mol[22], −169.0 kcal/kg (enthalpy of form.)[31], −25 ± 0.40 kcal/mol ($\Delta_f H^{298}$)[41], −20.13 kcal/mol ($\Delta_f H$)[41], −103.7 kJ/mol (enthalpy of form., exptl.)[42], −88.5 kJ/mol (enthalpy of form., calcd., emp.)[42], −103.8 kJ/mol (enthalpy of form., calcd., S-D method)[42], −103.0 ± 1.5 kJ/mol ($\Delta H_f°$, (c))[45], −24.81 kcal/mol ($\Delta H_f°$)[46]
Heat of combustion	2,477 cal/g[13, 19, 21], 369 kcal/mol[21], 2,506 (Q_c^p)[20], 2,477 cal/g (@ C^p)[22], ΔQ_c = 369 ± 0.40 kcal/mol (exptl.)[41], heat of comb. = 369.7 kcal/mol (@ 1 atm.)[43]

	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{ex}U^o$ [kJ kg^{-1}]	4,995	4,648 (calcd., K-J)[4] 1,133 kcal/kg (@ 1.700 g cm^{-3}, calcd.) [H_2O vapor][31] 1,194 cal/g (calcd.)[36]	4,699 [H_2O (l)][1] 4,278 [H_2O (g)][1] 1,276 cal/g[13, 19, 21, 22] 981 kcal/kg[16] 1,100 kcal/kg [H_2O (g)][17]

			1,100 kcal/kg (@ 1.700 g cm^{-3}, calcd.) [H_2O vapor][31] 1,276 kcal/kg[37]
T_{ex} [K]	3,187	4,300 (calcd.)[19]	
$p_{C\text{-}J}$ [kbar]	29.97	26.72 GPa (calcd., K-J)[2] 231 (calcd.)[19] 229 (@ 1.663 g cm^{-3} calcd., empirical, *Xiong*)[27] 242 (@ 1.532 g cm^{-3}, calcd., K-J)[28] 252 (@ 1.562 g cm^{-3}, calcd., K-J)[28]	273[9] 265.9[19] 266 (@ 1.532 g cm^{-3})[28] 273 (@ 1.562 g cm^{-3})[28]
VoD [m s^{-1}]	8,336 (@ 1.75 g cm^{-3}, $\Delta_f H = -103.834$ kJ mol^{-1})	7,890 (@ 1.65 g cm^{-3}, calcd., K-J)[2] 6,368 (@ 0.98 g cm^{-3}, calcd., BKWR)[25] 6,029 (@ 0.98 g cm^{-3}, calcd., BKWS)[25] 7,620 (@ 1.5 g cm^{-3}, average lit. value)[24] 8,391 (@ 1.710 g cm^{-3}, calcd.)[21] 8,310 (@ 1.71 g cm^{-3} (TMD), calcd., R-P method)[26] 8,640 (@ 1.71 g cm^{-3} (TMD), calcd., *Aizenshtadt*)[26] 8,280 (@ 1.71 g cm^{-3} (TMD), calcd., K-J)[26] 8,179 (@ 1.663 g cm^{-3}, calcd., empirical, *Xiong*)[27]	7,639 (@ 1.532 g cm^{-3}, pressed)[19] 7,570 (@ 1.65 g cm^{-3})[1, 15] 8,230 (@ 1.71 g cm^{-3})[10] 7,570 (@ 1.49 g cm^{-3}, 1.0 in charge diameter, pressed, unconfined)[13, 20] 7,680 (calcd. based on sand test with 1,700 g bomb)[24] 7,570 (@ 1.49 g cm^{-3}, pressed, unconfined, 1.0 diameter)[21] 7,580 (@ 1.50 g cm^{-3}, *Blatt*)[21, 22] 5,650 (@ 1.0 g cm^{-3}, *Blatt*)[21, 22] 6,600 (@ 1.25 g cm^{-3}, *Fischeroulle*)[21]

			7,137 (@ 1.50 g cm^{-3}, *Fischeroulle*)[21] 7,883 (@ 1.55 g cm^{-3})[22] 8,235 (@ 1.663 g cm^{-3})[27] 24,000–25,400 ft/s (@ 1.5 g/mL)[34] 7,750 (@ 1.55 g cm^{-3})[37] 7,550 (@ 1.50 g cm^{-3})[43]
V_0 [L kg^{-1}]	860		1,017[1, 14] 908[13, 20, 21, 37]
I_{sp} [Ns g^{-1}]	2.46 (calcd., ISPBKW code)[46], 2.48 (calcd., empirical)[46]		

Trauzl test [cm^3, % TNT]	122–143% TNT[22], 122% TNT[11, 13, 20, 21], 118% PA[21], 410[40]
Sand test [g]	48.4 g sand crushed (1,700 g bomb)[24], 52.3 g sand crushed (cf. 48 g for TNT) (109% TNT)[11, 13, 20, 21], 109–119% TNT[22]
Ballistic mortar test	136–140% TNT[22], 139% TNT[11, 13, 20, 21, 43], 136% TNT[21]
Initiation efficiency	0.21 g MF minimum detonating charge[13, 22], 0.13 g LA minimum detonating charge[13, 22, 38]
US NOL gap test	Gap value = 6.35 cm (@ 1.551 g cm^{-3}, pressed)[19]
Gap test	14 cm distance between two paper cartridges each containing 50 g EDNA of ρ = 0.80 g cm^{-3}[21, 22]
LSGT [cm]	60 mm (NOL)[30] ρ = 1.551 g/cc, 90.7% TMD, 50% point no. cards 250, regular test, charge conditioned and fired @ 25 °C[39]
1 s explosion T [°C] 5 s explosion T [°C] 10 s explosion T [°C] 5 s ignition T [°C] Dec. T [°C] Explosion T [°C]	216[20] 189 (dec.)[13, 20], 189 (detonates)[11], 189 (dec., cook-off)[38] 178[13, 20, 38] 189 (dec., USA value)[19, 38], 190 (Russian value)[19] 20 s @ 170[21], 15 s @ 173[21], 10 s @ 178[21], 5 s @ 189[21] 265 (0.1 s, no cap used)[13, 21, 22], 216 (1 s, no cap used)[13, 21], 205 (1 s, Blatt)[21], 265 (0.1 s)[38], 216 (1 s)[38]

<table>
<tr><td></td><td>Ignition or deflagration occurred, 25 mg sample: 0.166 sec. exposure time @ 314[21], 0.45 s exposure time @ 251[21], 1.18 s exposure time @ 203[21], 4.88 s exposure time @ 180[21], 37.1 s exposure time @ 162[21], 120 s exposure time @ 158[21], 793 s exposure time @ 149[21], no action @ 142[21]
190[22], explodes @ 180 °C on heating[29], 173 (15 s)[13], 170 (20 s)[13]

T (°C), time to explosion (s), 25 mg sample[33]:

<table>
<tr><th>T (°C)</th><th>Time to explosion (s)</th><th>T (°C)</th><th>Time to explosion (s)</th></tr>
<tr><td>314</td><td>0.166</td><td>180</td><td>4.88</td></tr>
<tr><td>286</td><td>0.242</td><td>176</td><td>6.80</td></tr>
<tr><td>266</td><td>0.333</td><td>169</td><td>13.5</td></tr>
<tr><td>251</td><td>0.450</td><td>162</td><td>37.1</td></tr>
<tr><td>232</td><td>0.554</td><td>158</td><td>120</td></tr>
<tr><td>221</td><td>0.750</td><td>149</td><td>793</td></tr>
<tr><td>192</td><td>2.08</td><td>142</td><td>No explosion</td></tr>
</table>
</td></tr>
<tr><td>International heat test</td><td>0.01% mass loss in 48 h @ 75 °C[20]</td></tr>
<tr><td>100 °C heat test [% mass loss]</td><td>0.2% mass loss in first 48 h[13, 20, 22], 0.3% mass loss in second 48 h[13, 20, 22], no explosions occurred in 100 h[13, 20, 22]</td></tr>
<tr><td>75 °C int. heat test</td><td>0.01% mass loss in 48 h[13, 22]</td></tr>
<tr><td>Thermal stability</td><td>Dry EDNA unaffected after 5 months storage @ 65 °C[11, 22], dry EDNA unaffected after 30 months storage @ 50 °C[11, 22], withstands 120 °C stability test as well as tetryl[29], dry EDNA is thermally stable but moisture causes dec. @ T > 50 °C[37]</td></tr>
<tr><td>Vacuum stability test [cm^3/h]</td><td>0.5 g cm^3 gas evolved @ 100 °C in 48 h (5 g sample)[22], 1.5–2.4 cc/48 h @ 120 °C (5 g sample)[22], 11 + cc/48 h @ 135 °C (5 g sample)[22], 1.5 cm^3 @ 120 °C, 40 h[38], 0.5 cc gas evolved in 40 h @ 100 °C[13, 20], 1.5 cc gas evolved in 40 h @ 120 °C[13, 20], 11+ cc gas evolved in 40 h @ 150 °C[13, 20], 0.5 cc/5 g in 48 h @ 100 °C[21], 1.5 cc/5 g in 48 h @ 120 °C[21], 11+ cc/5 g in 48 @ 135 °C[21], 5 mL gas (max.) in 40 h @ 120 °C (>90% purity)[22]</td></tr>
<tr><td>Volatility</td><td>0[13, 20, 21], 0.05%/h @ 100 °C in open dish[22]</td></tr>
</table>

<table>
<tr><td>Solubility [g/mL]</td><td>Solubility values (g/100 g solvent)[13]:
<table><tr><td colspan="2">Water</td><td colspan="2">Alcohol</td></tr><tr><td>°C</td><td>%</td><td>°C</td><td>%</td></tr><tr><td>20</td><td>0.25</td><td>20</td><td>1.00</td></tr><tr><td>40</td><td>0.75</td><td>40</td><td>2.46</td></tr><tr><td>60</td><td>2.13</td><td>60</td><td>5.29</td></tr><tr><td>80</td><td>6.38</td><td>78</td><td>10.4</td></tr><tr><td>100</td><td>> 20</td><td></td><td></td></tr></table>
Solubility in water (100 g): 0.10 g @ 10 °C, 0.25 g @ 20 °C, 1.25 g @ 50 °C, 5.0 g @ 75 °C, 16.4 g @ 95 °C[22]. Solubility in 95% EtOH (100 g): 0.55 g @ 10 °C, 1.00 g @ 20 °C, 3.50 g @ 50 °C, 10.07 g @ 75 °C, 11.5 g @ 78.5 °C[22], insoluble in Et_2O[22], 8.2 g dissolve in 100 g acetone @ 20 °C[22], soluble in nitromethane, nitrobenzene and dioxane[22], sparingly soluble in H_2O: ~ 1 part per 200 parts H_2O @ 25 °C[29], soluble in H_2O, EtOH, MeOH and acetone[34], soluble in nitrobenzene, dioxane, EtOH and boiling water[37], insoluble in Et_2O[37]

Data from[37]:
<table><tr><td rowspan="2">T (°C)</td><td colspan="2">Solubility g/100 g solvent</td></tr><tr><td>Water</td><td>Ethyl alcohol</td></tr><tr><td>25</td><td>0.3</td><td>1.25</td></tr><tr><td>50</td><td>1.25</td><td>3.45</td></tr><tr><td>75</td><td>4.95</td><td>10.1</td></tr><tr><td>95</td><td>16.4</td><td>–</td></tr></table></td></tr>
<tr><td>Hygroscopicity</td><td>Virtually nonhygroscopic absorbs only 0.01% moisture @ 30 °C with 90% RH[11], 0.01%[13], 0.01% @ 90% RH[22], slightly hygroscopic[34], may hydrolyze slightly in presence of H_2O[34], nonhygroscopic[37]</td></tr>
<tr><td>Compatibility</td><td>Dry EDNA does not react with most metals[11], reacts with brass, cadmium, copper, nickel, mild steel and zinc if moist[11]
Dry: Cu, brass, Al, mild steel, stainless steel, mild steel coated with acid-proof black paint, mild steel plated with copper nickel, cadmium or zinc are unaffected[13], Mg and Mg–Al alloy are slightly affected[13]
Wet: Cu, brass, Al, mild steel coated with acid-proof black paint, mild steel plated with copper, cadmium, nickel or zinc are heavily corroded[13], Al is slightly affected[13], stainless steel is unaffected[13]</td></tr>
</table>

	May hydrolyze slightly in presence of H_2O[34], when dry does not react with most common metals[34], reacts with most common metals (considerable corrosion) except Al and stainless steel in the presence of moisture[34], dec. on addition to hot dil. sulfuric acid[13], dec. by addition to excess 20% aq. NaOH soln.[13] Dry EDNA: no corrosion of Al, brass, Cu, mild steel, stainless steel, Cd, Ni or Zn[22], mild corrosion of Mg and Mg alloys[22], wet EDNA (≥0.5% moisture) heavily corrodes Cu, brass, mild steel, Cd, Ni and Zn[22], wet EDNA does not corrode stainless steel[22], stable in alkaline soln. but dec. in acid and neutral soln.[37]
Rifle bullet impact test	0% explosions, 60% partial detonations, 20% burned, 20% unaffected[13, 22], 90 (% detonations, pressed sample, reg disk bomb, 3/16 in steel disk)[43], 100 (% detonations, pressed sample, Reg disk bomb, 3/16 in steel disk)[43]
Plate dent test	Brisance = 122% TNT, $\rho = 1.49$ g cm^{-3}, charge diameter = 1.0 in, pressed, unconfined[13], 133–122% TNT[22]
Plate cutting test	Brisance equal to that of TNT[22]
Booster sensitivity test	Condition = pressed, 100 g tetryl, 2.09 in wax for 50% detonation, $\rho = 1.42$ g cm^{-3}[13, 38], pressed EDNA, $\rho = 1.42$ g cm^{-3}, 50% gap = 2.09 in[38]
Fragmentation test	3 in HE, M42A1 projectile, lot KC-5: 95:5 EDNA:wax, $\rho = 1.56$ g cm^{-3}, total no. of fragments = 514, total no. of fragments for EDNA = 600 (117% as many fragments as TNT)[13, 22], 136–147% as many fragments as TNT[22]
Heat of decomposition [cal/g]	573 (est.)[36]
Flash point [°C]	180[37]
C_p [cal mol^{-1} K^{-1}]	$C_p^{298} = 41.9$[41]

	EDNA[35]
Chemical formula	$C_2H_6N_4O_4$
Molecular weight [g mol^{-1}]	150.09
Crystal system	Orthorhombic
Space group	*Pbca* (61)
a [Å]	10.67
b [Å]	8.67
c [Å]	6.16
α [°]	90
β [°]	90

γ [°]	90
V [Å^3]	
Z	4
ρ_{calc} [g cm^{-3}]	
T [K]	

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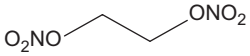
Ethylene glycol dinitrate

Name [German, acronym]: Ethylene glycol dinitrate, nitroglycol, dinitroglycol, dinitromethylene, ethylene dinitrate, glycol dinitrate [EGDN, EGcDN, NGc, NGL, GDN]

Main (potential) use: Secondary (high) explosive, ingredient of nonfreezing dynamite[2, 17]

Structural formula:



	Ethylene glycol dinitrate
Formula	$C_2H_4N_2O_6$
Molecular mass [g mol^{-1}]	152.06
Appearance at RT	Transparent liquid[15], colorless liquid[16], slightly syrupy liquid[24], yellow liquid[2], yellow oily liquid[26], transparent, free-flowing liquid[27]
IS [J]	1, 20–25 cm with 2 kg mass[4], FI = 20% PA[9], 110 cm (minimum fall, 5 kg mass, B.M.)[9], 20–25 cm (sample absorbed on filter paper, 2 kg mass, Kast app.)[9, 16], 4 in (20 mg sample, 1 lb mass, P.A.)[9], steel weight of 1 kg tests positive for all heights[7], DH_{50} = 3.763 cm (0.3542 kg, Bruceton method)[7], DH_{50min} = 2.810 cm (0.3542 kg, Bruceton method)[7], E_{min} = 0.099 (0.3542 kg, Bruceton method)[7], E_{max} = 0.133 (0.3542 kg, Bruceton method)[7], explodes on 2 kg mass falling 20–25 cm[15], 110 cm (500 g mass, Rinkenbach using small drop machine)[16], 0.2 Nm[19], 4 cm (1 lb mass, 20 mg sample, B.M.)[2], explodes if 2 kg mass is dropped from 10–12 cm[27], 20–25 cm (2 kg mass)[30], $H_{100\%}$ = 7 cm (5 kg mass, 10–11 °C, 0.1 g sample)[30]
FS [N]	>360, very sensitive[30], detonates when ground in porcelain mortar[30], all samples detonate in 10 friction pendulum tests[30]
N [%]	18.42
Ω(CO_2) [%]	0.00
$T_{m.p.}$ [°C]	−22[23], −21.7 (freezing point)[27], −22.3 or −22.8 (freezing point)[15], −22.3 (freezing point)[16], −23[19], −22.8[21], −22.3[25], −20[2], −22.3 – −22.80 (freezing point)[30]
$T_{b.p.}$ [°C]	197.5[15, 30], 105.5 (@ 19 mm Hg)[15], 70 (@ 2 mm Hg)[15]
$T_{dec.}$ [°C]	184.51 (onset), 189.36 (max.) (DSC @ 1 °C/min)[7], 191.93 (onset), 202.73 (max.) (DSC @ 3 °C/min)[7], 199.88 (onset), 208.8 (max.) (DSC @ 5 °C/min)[7], 201.01 (onset), 214.12 (max.) (DSC @ 8 °C/min)[7], explodes @ 215 °C if rapidly heated[9], 78 (TGA midpoint)[19]

ρ [g cm^{-3}]	1.489 (@ 2 °C)[4, 30], 1.481 ((l), @ 298 K)[2], sp. gr. = 1.488 (@ 20/4°)[9], sp. gr. = 1.480 (@ 25°)[9], 1.5176 (@ 0 °C)[15], 1.496 (@ 15 °C)[15], 1.489 (@ 20 °C)[15], d_4^{20} = 1.4918[16], sp. gr. (X°/15°) = 1.5176 (@ 0°)[16], sp. gr. (X°/15°) = 1.5033 (@ 10°)[16], sp. gr. (X°/15°) = 1.4890 (@ 20°)[16], 1.489[20], 1.49[21], 1.492 (pycnometry)[23], sp. gr. = 1.496[24], 1.48 (liquid)[2], sp. gr. = 1.491 (25/4 °C)[26], sp. gr. $d^{20°}_{20°}$ = 1.489[27]		
Heat of formation	−55.58 kcal/mol[9], −67.7 kcal/mol ($\Delta_f H$)[15], −382 kJ/kg (enthalpy of form.)[18], −243.01 kJ/mol[23], −366 cal/g[2], −1,529.3 J/g (@ constant volume)[30], −229.3 kJ/mol (@ constant volume)[30], 283.26 kJ/mol ($-\Delta_f H$)[30], −232.6 kJ/mol (enthalpy of form., exptl.)[31], −282.5 kJ/mol (enthalpy of form., calcd., emp.)[31]		
Heat of combustion	1,764 cal/g[2], 1,763.9 cal/g (@ C^v)[9], 268.22 kcal/mol (@ C^v)[9], 1,752.5 cal/g (@ C^p)[9], 266.48 kcal/mol (@ C^p)[9], 7,380.6 J/g (@ constant volume)[30], 7,334.6 J/g (@ constant pressure)[30]		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]	6,563	1,580.9 cal/g [H_2O (g)][9] 1,705.3 cal/g [H_2O (l)][9] 1,615 kcal/kg (@ 1.492 g cm^{-3}, calcd.) [H_2O vapor][18] 7,289 J/g [H_2O (l)] (calcd., ICT Thermodynamic code)[19] 1,655 kcal/kg[27] 176.6 kcal/100 g (@ 1.496 g cm^{-3}, constant volume) [H_2O (l)][28]	1,620 kcal/kg [H_2O (g)][3] 6,610.72 J/g [H_2O (g)][4, 30] 7,133.72 J/g [H_2O (g)][4] 1,578 kcal/kg [H_2O (g)][5] 1,580 kcal/kg [H_2O (g)][15] 1,705 kcal/kg [H_2O (l)][15] 1,578 kcal/kg (@ 1.492 g cm^{-3}) [H_2O vapor][18] 7,133.72 [H_2O (l)][30]
T_{ex} [K]	4,541	4,209 °C[9] 5,090 (calcd.)[8] 4,830 °C (@ 1.496 g cm^{-3})[28] 4,553 K[30]	

$p_{C\text{-}J}$ [kbar]	212	200 (calcd.)[8] 20.37 GPa (@ 1.492 g cm^{-3} (pycnometry density), heat of formation = −243.01 kJ/mol, CHEETAH 6.0)[23] 3.594 (@ 0.69 g cm^{-3} (SSED density), heat of formation = −243.01 kJ/mol, CHEETAH 6.0)[23]	
VoD [m s^{-1}]	7,576 (@ TMD)	7,490 (@ 1.48 g cm^{-3} (TMD), calcd., R-P method)[13] 7,500 (@ 1.5 g cm^{-3}, calcd.)[8] 7,517 (@ 1.492 g cm^{-3} (pycnometry density), heat of formation = −243.01 kJ/mol, CHEETAH 6.0)[23] 4,198 (@ 0.69 g cm^{-3} (SSED density), heat of formation = −243.01 kJ/mol, CHEETAH 6.0)[23] 7,300 (@ 1.485 g cm^{-3})[30] EGDN can detonate with high or low velocity[15]	7,300 (@ 1.48 g cm^{-3})[1, 14] 7,360 (@ 1.50 g cm^{-3})[3] 7,780 (0.36 loading diameter, steel tube 2.5 mm wall thickness, direct initiation by no. 8 detonator)[4] 7,960 (0.38 loading diameter, steel tube 2.5 mm wall thickness, 80 g mandelic acid as booster charge and directly by no. 8 detonator)[4] 8,100 (0.45 loading diameter, steel tube 2.5 mm wall thickness, 80 g mandelic acid as booster charge and directly by no. 8 detonator)[4] 1,830 (0.60 loading diameter, porcelain crucible, open, directly by no. 8 detonator)[4] 7,980 (0.60 loading diameter, porcelain crucible, cool down to −70 °C, directly by no. 8 detonator)[4] 7,400 (@ 1.5 g cm^{-3})[8] 7,390[6] 7,300 (@ 1.485 g cm^{-3}, liq., glass tubes, 1 cm diameter, 1 mm wall thickness)[9] 1,600–1,900 (@ 1.6 g cm^{-3}, liq., glass tubes, 0.39 in diameter)[9] 7,700 (@ 1.485 g cm^{-3}, liq., steel tube, 1.15 in diameter)[9]

7,830 (liq., loaded in iron pipe, 32–38 mm diameter, initiated by No. 8 detonator)[15]

8,200–8,300 (liq., loaded in iron pipe, 32–38 mm or 35–43 in diameter, initiated by 80 g PA)[15]

1,000–3,000 (liq., loaded in crucible, initiated by No. 8 detonator)[15]

>8,000 (solid, –70 °C, loaded in crucible, initiated by No. 8 detonator)[15]

Correlation between the detonation velocity of glycol dinitrate and the loading condition, data from[30]:

Loading condition/ method	Material of Container	Initiation approach	Detonation velocity (m/s)
Loading diameter φ36 mm	Seamless steel tube (2.5 mm wall thickness)	Directly by #8 detonated	7,780
Loading diameter φ38 mm	Seamless steel tube (2.5 mm wall thickness)	80 g mandelic acid as Booster charge, and directly by #8 Detonated	7,960
Loading diameter φ45 mm	Seamless steel tube (2.5 mm wall thickness)	80 g mandelic acid as booster charge, and directly by #8 detonated	8,100
φ60 mm porcelain crucible	Open	Directly by #8 detonated	1,830
φ60 mm porcelain crucible	Cool down to –70 °C	Directly by #8 detonated	7,980

V_0 [L kg^{-1}]	811	483 (without H_2O @ 25 °C)[19] 737[27] 73.7 l/100 g (@ 1.496 g cm^{-3}, @ STP)[28] 737.2[30]	

Detonation failure diameter, d_f [mm]	1.9 mm (neat EGDN in glass capillaries)[20]
Trauzl test [cm^3, % TNT]	600 cc (10 g sample with water tamping, cf. 590 cc for NG), 110% NG[9], 170% PA[9], 650 cm^3 (i.e., 110% NG) (H_2O tamping)[15, 16, 30], 600 cc[27], 620[29]
Sand test [g]	62.7 g[30]
Lead cylinder	Brisance = 22–24 mm compression[30]
5 s explosion T [°C] 5 s ignition T [°C] Explosion T [°C] Autoignition T [°C]	257[2, 9, 30e] 237[8] heating to 195–200 usually provokes an explosion[15], 195–200[30] 270[26]
100 °C heat test [% mass loss]	Usually fails heat test @ 72 °C[15]
Abel test	30 min (heat resistance)[30]
Thermal stability	4.2% began to dec. in 12 days @ 75 °C, 35.0% in 18 days @ 75 °C (loosely covered weighing dish)[9], no dec. after 260 h @ 75 °C[30]
Vapor pressure [atm. @ °C]	0.0044 mm Hg @ 0 °C[2], 0.038 mm Hg @ 20 °C[2], 0.26 mm Hg @ 40 °C[2], 1.3 mm Hg @ 60 °C[2], 5.9 mm Hg @ 80 °C[2], 22.0 mm Hg @ 100 °C[2], 0.031 Torr @ 15 °C[10], 0.058 Torr @ 22 °C[10], 0.078 Torr @ 25 °C[10], 0.196 Torr @ 35 °C[10], 0.448 Torr @ 45 °C[10], 0.648 Torr @ 50 °C[10], 0.26 Torr @ 40 °C[11], 1.3 Torr @ 60 °C[11], 5.9 Torr @ 80 °C[11]

T [°C]	Vapor pressure (Torr)[12]
15	0.23[12]
22	0.053[12]
25	0.71[12]
35	0.219[12]
45	0.443[12]
50	0.652[12]

T [°C]	Vapor pressure (mm Hg)[9]
22	0.0565[9]
20	0.0490[9]
50	0.0665[9]
15	0.02330[9]
25	0.07059[9]
35	0.2190[9]
45	0.44250[9]
55	0.9619[9]

0.3 mm Hg @ 20 °C (*Moreschi*)[15], 0.0565 mm Hg @ 22 °C (*Rinkenbach*)[15]

Vapor pressure values from *Marshall* cited in[15]:

Vapor pressure (mm Hg)[15]	*T* (°C)
0.0044	0
0.038	20
0.26	40
1.3	60
5.9	80
22.0	100

Vapor pressure values from *Bronder* cited in[15]:

Vapor pressure (mm Hg)[15]	*T* (°C)
0.048	20
0.125	30
0.299	40
0.648	50

<table>
<tr>
<td></td>
<td>0.07 mm Hg @ 0 °C[16], 0.0565 mm Hg @ 22 °C[16], 0.0706 Torr @ 25 °C[21], 1.2 × 10^5 ppb_v (equilibrium vapor pressure @ 300 K)[22], 7.2 × 10^{-2} mm Hg @ 25 °C[25], 0.030 mm Hg @ 15 °C[26], 0.040 mm Hg @ 20 °C (est.)[26], 0.072 mm Hg @ 25 °C[26], 0.180 mm Hg @ 35 °C[26], saturated air contains 95 ppm vapor by volume @ 25 °C and 760 mm Hg[26]
<table>
<tr><th>T (°C)</th><th>Vapor pressure (mm Hg)[27]</th></tr>
<tr><td>0</td><td>0.044</td></tr>
<tr><td>20</td><td>0.038</td></tr>
<tr><td>40</td><td>0.26</td></tr>
<tr><td>60</td><td>1.3</td></tr>
<tr><td>80</td><td>5.9</td></tr>
<tr><td>100</td><td>22.0</td></tr>
</table>
<table>
<tr><th>T (°C)</th><th>Vapor pressure (mm Hg)[30]</th></tr>
<tr><td>0</td><td>0.0044</td></tr>
<tr><td>20</td><td>0.046</td></tr>
<tr><td>30</td><td>0.125</td></tr>
<tr><td>40</td><td>0.289</td></tr>
<tr><td>50</td><td>0.735</td></tr>
<tr><td>60</td><td>1.302</td></tr>
<tr><td>70</td><td>3.986</td></tr>
<tr><td>80</td><td>5.976</td></tr>
<tr><td>90</td><td>13.972</td></tr>
<tr><td>100</td><td>22.062</td></tr>
</table>
</td>
</tr>
<tr>
<td>Volatility</td>
<td>Mass loss from 15 g sample (open dish, 65 mm diameter, 40 mm high)[9, 30]:
@ 20 °C: 0.14% after 24 h[9, 30], 0.37% after 48 h[9, 30], 1.63% after 7 days[9, 30], 2.06% 0.37% after 12 days[9, 30], 6.91% after 30 days[9, 30], 47.0% after 6 months[9, 30]
@ 35 °C: 3.6% after 24 h[9, 30], 8.1% after 48 h[9, 30], 21.7% after 7 days[9, 30], 46.6% after 12 days[9, 30], 68.5% after 20 days[9, 30], 100% after 40 days[9, 30]

2.2 mg/cm^2/h[15], 20 times more volatile than NG[30], 2.2 mg/cm^2/h@ 60 °C[30]</td>
</tr>
</table>

Viscosity [Poises]	4.2 @ 20 °C[2, 30], 0.0421 @ 20 °C[9], 0.0214 @ 50 °C[9], 0.0363 @ 20 °C[9], 0.08056 @ 15 °C[15, 30], 0.02831 @ 40 °C[15, 30], 0.0363 @ 23.6 °C[15, 30], 0.042 @ 20 °C[15, 30], η_{20} = 4.61 cP[15, 16], only slightly more viscous than H_2O[16], 4 cP[27]
Index of refraction	1.4452 @ 22.3 (for white light)[16], 1.4713 @ 22.3 (for white light, commercial sample)[16]
Dielectric constant	ε_{20} = 28.26[15, 16]
Dipole moment, μ [D]	4.00[15, 16, 30], 3.28 (soln. in benzene)[30]
Burn rate [mm/s]	cannot be burned under pressure of 230 mm Hg but is easily detonated (4 mm diameter glass tube, 14–15 °C)[30]
Flame sensitivity	ignites with hissing on contact with flame while local overheating may result in explosion[27], very sensitive[30], stable combustion @ atmospheric pressure in contact with flames[30]
Solubility [g/mL]	6.2 g/L H_2O @ 15 °C[2], 6.8 g/L H_2O @ 20 °C[2], 9.2 g/L H_2O @ 50 °C[2], fairly soluble in most common organic solvents[15], less soluble in CCl_4 and petrol[15], 0.62 g dissolves in 100 mL H_2O @ 15 °C[15], 0.68 g dissolves in 100 mL H_2O @ 20 °C[15], 0.92 g dissolves in 100 mL H_2O @ 50 °C[15], 0.57 g dissolves in 100 mL H_2O @ 0 °C[15] 6.2 g dissolves in 1 L @ 15 °C[16], 6.8 g dissolves in 1 L H_2O @ 20 °C[16], 9.2 g dissolves in 1 L H_2O @ 50 °C[16], aqueous solubility = 5,600 mg/L @ 25 °C[21], 5,200 mg/L in H_2O @ 25 °C[25], 0.45% (w/v) in water @ 21 °C[26], soluble in CCl_4, EtOH, acetone, benzene, toluene and methanol[26], slightly soluble in dil. alkali[26], readily soluble in tetryl and methyl alcohols, Et_2O, $CHCl_3$, acetone, benzene, nitrobenzene and toluene[27], poorly soluble in CCl_4[27], 0.52 g dissolves in 100 g H_2O @ 25 °C[27], 0.85 g dissolves in 100 g H_2O @ 60 °C[27], slightly soluble in water[30], soluble in most organic solvents[30], slightly soluble in CCl_4 and gasoline[30], solubility in water @ 20 °C is four times higher than that of NG[30] Solubility in water data from[30]: *T* (°C) | g EGDN/100 g H_2O 0 | 0.57 15 | 0.62 20 | 0.68 50 | 0.92 60 | 0.85

<table>
<tr><td></td><td>Solubility of EGDN in nitric acid, weight of EGDN dissolved (%)[30]:

<table>
<tr><td rowspan="2">T (°C)</td><td colspan="5">Concentration of nitric acid (%)</td></tr>
<tr><td>0</td><td>4.93</td><td>9.99</td><td>19.67</td><td>29.58</td></tr>
<tr><td>0</td><td>0.57</td><td>0.77</td><td>1.02</td><td>1.52</td><td>2.03</td></tr>
<tr><td>20</td><td>0.631</td><td>0.81</td><td>1.10</td><td>1.61</td><td>2.24</td></tr>
</table>
Solubility in aq. sodium carbonate soln. @ 20 °C[30]:

<table>
<tr><td>Na_2CO_3 content (%)</td><td>Solubility (%)</td></tr>
<tr><td>1.39</td><td>0.48</td></tr>
<tr><td>12.5</td><td>1.14</td></tr>
</table></td></tr>
<tr><td>Hygroscopicity</td><td>Nonhygroscopic[16, 30], 0.0% @ 30 °C, 90% RH[2], low hygroscopicity[27]</td></tr>
<tr><td>Compatibility</td><td>Readily gelatinized by collodion @ RT[27], readily hydrolyzed when heated with aq. NaOH or KOH soln.[30], vigorous reaction in contact with EtOH soln. of KOH[30], hydrolyzed in hot water[30], can dec. on contact with acid for prolonged periods of time[30]</td></tr>
<tr><td>Diffusion coefficient [cm^2/s]</td><td>0.084 (air)[21], 8.72×10^{-6} (water)[21]</td></tr>
<tr><td>Log K_{ow}</td><td>1.16[21, 25]</td></tr>
<tr><td>Log K_{oc}</td><td>1.28[21]</td></tr>
<tr><td>Refractive index</td><td>$n^D_{25} = 1.4452$[2]

<table>
<tr><td>T (°C)</td><td>0</td><td>15</td><td>25</td><td>35</td></tr>
<tr><td>Refractive index</td><td>1.4546</td><td>1.4491</td><td>1.4454</td><td>1.4417</td></tr>
</table></td></tr>
<tr><td>$\Delta H_{melting}$ [J/g]</td><td>125.52 (latent heat of melting)[30]</td></tr>
<tr><td>Closed bomb test</td><td>Gas vol. produced on explosion of 1 kg = 736.93 L (@ 0 °C and 760 mm Hg)[9], gas vol. produced on explosion of 1 kg calcd. to temperature of explosion 4,209 °C = 12,099 L[9], pressure developed on explosion of 1 kg in 1 L = 12,498 kg/cm^2[9]</td></tr>
</table>

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[31] B. Nazari, M. H. Keshavarz, M. Hamadanian, S. Mosavi, A. R. Ghaedsharafi, H. R. Pouretedal, *Fluid Phase Equilibria,* **2016**, *408*, 248–258.

Ethyl nitrate

Name [German, acronym]: Ethyl nitrate, ethanol nitrate
Main (potential) use: Improvised explosive, rocket propellants, has been used as an ingredient of liquid rocket fuels[9], component of liquid rocket fuel[20], in combination with other oxidants act as mixed explosives for engineering blasting[20]

Structural formula:

	Ethyl nitrate
Formula	$C_2H_5NO_3$
Molecular mass [g mol^{-1}]	91.07
Appearance at RT	Liquid[9], colorless liquid[10], transparent oily liquid with slightly aromatic odor[20]
IS [J]	2 kg @ 500 mm[4], $H_{50\%}$ = 50 cm (2 kg mass)[9], 1–2 kg cm (ERL apparatus)[11], 44 cm (median height, Rotter apparatus)[18], 50% explosion caused by dropping 2 kg mass from 50 cm[20]
FS [N]	>360
N [%]	15.38
Ω(CO_2) [%]	−61.49
$T_{m.p.}$ [°C]	−95[3], −102[5]
$T_{b.p.}$ [°C]	87[9, 10, 20], 86 (@ 760 mm Hg)[11], 87.5[12], 88[20]
$T_{dec.}$ [°C]	175 (exo, DSC @ 10 °C/min, sealed pan)[11]
ρ [g cm^{-3}]	1.11 (@ 293 K), 1.12[4, 20], 1.10[5, 11], sp. gr. = 1.044 (@ 25 °C)[6], sp. gr. = 1.116 (@ 15 °C)[6], sp. gr. = 1.12[9], sp. gr. = 1.1159 (15°/15°, @ 15°)[10], sp. gr. = 1.1044 (25°/25°, @ 25°)[10], sp. gr. = 1.105 @ 20 °C[12]
Heat of formation	−190.4 ± 1.2 kJ/mol ($\Delta_fH°$, liq.)[8], −122 ± 1.3 kJ/mol ($\Delta_fH°$, gas)[8], −37 kcal/mol ($\Delta_fH°$ gas)[1], −2,091 kJ/kg (enthalpy of form.)[5], 48.5 kcal/mol[6], 33.7 kcal/mol[6], −47 kcal/mol (Δ_fH)[11], −37.0 kcal/mol (Δ_fH, calcd. based on thermochemical data)[9], −45.7 kcal/mol (@ 25 °C, calcd., based on thermochemical data)[10, 15], 45.32 kcal/mol (calcd.)[15]
Heat of combustion	ΔH_c (est.) = −324.04 kcal/mol[9], Q_c = 313.59 kcal/mol (calcd.)[15], Q_c = 313.2 kcal/mol (obs.)[15], combustion heat = 1,347.25 kJ/mol[20], − $\Delta H_{combustion}$ = 1,355.78 kJ/mol[20]

	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{ex}U^{o}$ [kJ kg^{-1}]	4,712	816.3 kcal/kg (@ C^{V}, $\Delta_f H = 48.5$ kcal/mol) [H_2O (l)][6] 712.6 kcal/kg (@ C^{V}, $\Delta_f H = 48.5$ kcal/mol) [H_2O (g)][6] 5.17 MJ/kg (calcd., SD method)[17]	4,154 [H_2O (l)][5] 3,431–3,473 [H_2O (g)][3] 3,568.95 [H_2O (l)][20]
T_{ex} [K]	3,130	3,128 (calcd., SD method)[17]	
$p_{C\text{-}J}$ [kbar]	123	132 (calcd., TIGER)[11] 114 (calcd., K-J)[11]	
VoD [m s^{-1}]	6,321 (@ TMD)		6,000–7,000 (wide tubes, indirectly measured in $EtONO_2$/Kieselguhr mixtures)[4] 5,800 (@ 1.1 g cm^{-3}, confined)[5] 5,800 (steel tube, 27 mm diameter)[4] 6,020 (steel tube, 60 mm diameter)[4] 6,000–7,000 (in wider diameter tubes)[9] 5,800 (thick-walled metal tube, 27 mm inner diameter, detonated by ~40 g PETN)[9] 6,020 (thick-walled metal tube, 60 mm inner diameter, detonated by ~40 g PETN)[9] 6,010 (@ 1.11 g cm^{-3}, D_i; D_i = ideal detonation velocity, steel tube)[17]

			No detonation observed in steel tube of 10 mm[4] 6000–7000 in wide tubes (no ρ specified)[20] 5,800 in steel tube with 27 mm diameter (no ρ specified)[20] 6,020 in steel tube with 60 mm (no ρ specified)[20] Detonation did not occur in steel tube with 10 mm diameter[20]
V_0 [L kg^{-1}]	976		1,101[2, 5]

Trauzl test [cm^3, % TNT]	345 cc (10 g sample, initiated by No. 8 blasting cap, underwater tamping)[6], 345 cm^3 (H_2O tamping)[9, 20], ~20% greater than that of PA[9, 20], 420[19]
Sand test [g]	58% NG[10]
Ballistic mortar test	123% TNT[5, 6]
Initiation efficiency	Can be detonated in thick-walled metal tubes by ~40 g PETN[9], attempts to detonate in glass tubes (10 mm diameter) unsuccessful[9], not detonated by No. 8 blasting cap unless ethyl nitrate tamped or confined[10]
Gap test	Scale I (detonator = standard commercial No. 8 Briska type, donor = 2 × 20 g pellets of tetryl pressed to ρ = 1.5 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) critical card value = 2[14] Scale III (donor = 2 × 20 g pellets of tetryl pressed to ρ = 1.5 g ml, each 1.5 in in diameter, Gap = 4 in square cards, charge case = 3 in length of 1 ½ 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) critical card value = 43[14]

<table>
<tr><td></td><td>Probable critical card values[14]:
<table><tr><td>Card value</td><td>Probability</td><td>Card value</td><td>Probability</td></tr><tr><td>41</td><td>0.021</td><td>44</td><td>0.316</td></tr><tr><td>42</td><td>0.135 > 44</td><td>0.071</td><td></td></tr><tr><td>43</td><td>0.458</td><td></td><td></td></tr></table></td></tr>
<tr><td>5 s explosion T [°C]</td><td>Explosive dec. on superheating[12]</td></tr>
<tr><td>Vapor pressure [atm. @ °C]</td><td>Exptl. determined values[9]:
<table><tr><td>Vapor pressure (mm Hg)</td><td>T (°C)</td></tr><tr><td>16.3</td><td>0</td></tr><tr><td>49.9</td><td>20</td></tr><tr><td>81.8</td><td>30</td></tr><tr><td>129</td><td>40</td></tr><tr><td>197</td><td>50</td></tr><tr><td>292</td><td>60</td></tr></table>64 mm @ 25 °C[11], 0.93 atm. @ 85.5 °C[16], 1.22 atm. @ 94.0 °C[16], 1.80 atm. @ 103.8 °C[16], 2.24 atm. @ 112.5 °C[16], 3.40 atm. @ 128.3 °C[16], 5.10 atm. @ 144.0 °C[16], 6.80 atm. @ 159.0 °C[16], 10.20 atm. @ 177.0 °C[16], 13.61 atm.@ 190.5 °C[16]</td></tr>
<tr><td>Enthalpy of vaporization [kJ mol^{-1}]</td><td>36.3 ± 0.4 ($\Delta_{v,s}H°$)[8], latent heat of evaporation (ΔH_v) @ 25 °C = 8.7 kcal/mol (calcd. based on thermochemical data)[9]</td></tr>
<tr><td>Solubility [g/mL]</td><td>Scarcely miscible with H_2O[9] readily dissolved by common organic solvents[9], soluble in water, EtOH and Et_2O[12], slightly soluble in water[20], miscible with alcohols and most organic solvents[20]</td></tr>
<tr><td>Wedge test</td><td>>100% PETN energy in donor required to initiate EN in a long, thin wedge @ 1/8 in thickness in receptor end[11]</td></tr>
<tr><td>Flame T [K]</td><td>1,470 ((g) @ 0.1 MPa)[13]</td></tr>
</table>

[1] M. Jaidann, D. Nandlall, A. Bouamoul, H. Abou-Rachid, *Defence Research Reports*, DRDC-RDDC-2014-N35, 12th March **2015**.

[2] M. Jafari, M. Kamalvand, M. H. Keshavarz, A. Zamani, H. Fazeli, *Indian J. Engineering and Mater. Sci*., *22*, **2015**, 701–706.

[3] W. C. Lothrop, G. R. Handrick, *Chem. Revs*., **1949**, *44*, 419–445.

[4] J. Liu, *Liquid Explosives*, Springer-Verlag, Heidelberg, **2015**.

[5] R. Meyer, J. Köhler, A. Homburg, *Explosives*, 7th edn., Wiley-VCH, Weinheim, **2016**, p. 128.

[6] B. T. Fedoroff, O. E. Sheffield, *Encyclopedia of Explosives and Related Items*, *vol. 6*, US Army Research and Development Command, TACOM, Picatinny Arsenal, USA, **1974**.
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[10] T. L. Davis, *The Chemistry of Powder and Explosives*, *vol. 2*, **1943**, John Wiley and Sons Inc., New York, pp. 194–195.
[11] M. E. Hill, J. M. Guimont, *Desensitization of Explosive Materials*, ADA082893, Office of Naval Research, Maryland, USA, April 9th **1980**.
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[13] N. Kubota, *Propellants and Explosives: Thermochemical Aspects of Combustion*, Wiley, **2002**.
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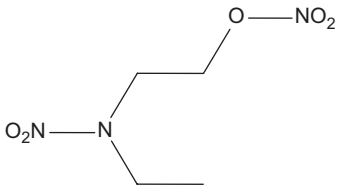
[16] A. G. Whittaker, *Rev. Scientific Instr.*, **1957**, *28*, 360–364.
[17] G. D. Kozak, *Combust. Expl. Shock Waves*, **1998**, *34*, 581–586.
[18] *Services Textbook of Explosives*, JSP 333, Procurement Executive, Ministry of Defence, UK, March **1972**.
[19] M. Jafari, M. Kamalvand, M. H. Keshavarz, S. Farrashi, *ZAAC*, **2015**, *641*, 2446–2451.
[20] J. Liu, *Nitrate Esters Chemistry and Technology*, Springer, **2019**.

N-Ethyl-*N*-(2-nitroxyethyl)nitramine

Name [German, acronym]: *N*-Ethyl-*N*-(2-nitroxyethyl)nitramine, 1-(*N*-ethyl)-nitramino-2-ethanol nitrate, *N*-(β-nitroethyl)-ethylnitramine, *N*-(2-nitratoethyl)-ethylnitramine, 2-[ethyl(nitro)amino]ethyl nitrate, ethyl-2-nitratoethyl nitramine [EtNENA]

Main (potential) use: Plasticizer for propellant applications[1, 8]

Structural formula:



	EtNENA		
Formula	$C_4H_9N_3O_5$		
Molecular mass [g mol^{-1}]	179.13		
Appearance at RT	Liquid[6, 7, 8], pale yellow oil		
N [%]	23.46		
Ω(CO_2) [%]	−67.0		
$T_{m.p.}$ [°C]	4–5.5[2, 3], 5[1, 7], 1–5[4, 5], 1[6], 2–4 (freezing point)[8]		
$T_{dec.}$ [°C]	210 (exo, DSC)[4, 5]		
ρ [g cm^{-3}]	1.32 (@ 298.15 K)[2], sp. gr. = 1.32 (@ 25/4°)[2, 3], 1.32[4, 5, 6]		
Heat of formation	−177.9 kJ/mol (enthalpy of form.)[1], −993.14 kJ/kg (enthalpy of form.)[1], 784 kJ/mol ($\Delta_f H$)[4, 5], −39.204 cal/mol ($\Delta_f H$)[6]		
	Calcd. (EXPLO5_V6.05.02)	Lit. values	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]	4,882	784 cal/g (@ 0.20 g/cc, calcd., Blake code)[6] 784 cal/g (calcd.)[7]	
T_{ex} [K]	3,106	2,461 (@ 0.20 g/cc, calcd., Blake code)[6]	

$p_{C\text{-}J}$ [GPa]	15.8		
VoD [m s^{-1}]	6,858 (@ TMD)		
V_0 [L kg^{-1}]	889		

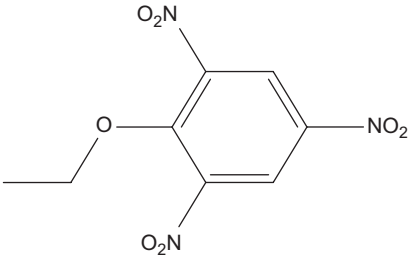
[1] R. Meyer, J. Köhler, A. Homburg, *Explosives*, 7th edn., Wiley-VCH, Weinheim, **2016**, pp. 128–129.
[2] A. T. Blomquist, F. T. Fiedorek, *Nitramines*, US Patent 2,485,855, 25th October **1949**.
[3] B. T. Fedoroff, O. E. Sheffield, *Encyclopedia of Explosives and Related Items*, *vol. 6*, US Army Research and Development Command, TACOM, Picatinny Arsenal, USA, **1974**.
[4] E. Rozumov, *Recent Advances in Gun Propellant Development: From Molecules to Materials*, in *Energetic Materials From Cradle to Grave*, M. K. Shukta, V. M. Bodelu, J. A. Steevens, R. Damavarapu, J. Leszczynski (eds.), Springer-Verlag, **2017**, pp. 23–65.
[5] A. Provatos, *Energetic Polymers and Plasticisers for Explosive Formulations – A Review of Recent Advances*, DSTO-TR-0966, DSTO, Melbourne, Australia, **2000**.
[6] R. L. Simmons, *Energetic Liquid Azido Nitramines*, ICT **1999**, Karlsruhe, Germany, 3-1–3-13.
[7] E. H. Zeigler, *Stable Plasticizers for Nitrocellulose/Nitroguanidine-Type Compositions*, European Patent EP 0 490 258 A1, 4th December **1991**.
[8] J. V. Urenovitsch, *Low Vulnerability Propellant Plasticizers*, US Patent 5482581, 9th January **1996**.

Ethyl picrate

Name [German, acronym]: 2-Ethoxy-1,3,5-trinitrobenzene, ethyl picrate, 2,4,6-trinitrophenetole, trinitrophenylethyl ether, picryl ethyl ether [ethylpikrat, pikrinsäureäthyläther, 2,4,6-TNPh^{i}t]

Main (potential) use: Component of explosive mixtures

Structural formula:



	Ethyl picrate		
Formula	$C_8H_7N_3O_7$		
Molecular mass [g mol^{-1}]	257.16		
Appearance at RT	Yellow crystals[10], light yellow solid[11], crystalline substance[12]		
N [%]	16.34		
Ω(CO_2) [%]	−77.8 [8]		
$T_{m.p.}$ [°C]	78[1]		
ρ [g cm^{-3}]	1.554 ± 0.06 (@ 293.15 K)[2], 1.52[3]		
Heat of formation	−200.8 kJ/mol (enthalpy of form., exptl.)[12], −222.2 kJ/mol (enthalpy of form., calcd., emp.)[12], −196.7 kJ/mol (enthalpy of form., calcd., S-D method)[12], −781 kJ/kg (enthalpy of form.)[3]		
Heat of combustion	936 kcal/mol (Q_c^V)[8]		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{ex}U^{\circ}$ [kJ kg^{-1}]	3,420 (calcd., K-J)[4]		3,515 [H_2O (l)][3, 6] 3,369 [H_2O (g)][3]
T_{ex} [K]			
$p_{C\text{-}J}$ [GPa]	16.9		

VoD [m s^{-1}]	6,844 (@ TMD)	6,310 (@ 1.60 g cm^{-3} (TMD), calcd. R-P method)[9] 6,500 (@ 1.55 g cm^{-3})[11]	6,500 (@ 1.55 g cm^{-3}, confined)[3] 6,800 (@ 1.60 g cm^{-3})[5] ~6,880[8]
V_0 [L kg^{-1}]	668		859[3, 7]

Trauzl test [cm^3, % TNT]	Almost as powerful as TNT, slightly less powerful than PA[8]

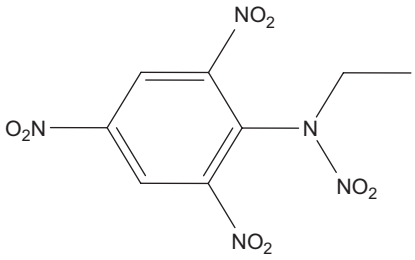
[1] R. C. Farmer, *J. Chem. Soc.,* **1959**, 3430–3433.
[2] Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© **1994–2017** ACD/Labs).
[3] R. Meyer, J. Köhler, A. Homburg, Explosives, 7th edn., Wiley-VCH, Weinheim, **2016**, pp. 129–130.
[4] M. H. Keshavarz, *Thermochimica Acta,* **2005**, *428*, 95–99.
[5] M. H. Keshavarz, *Propellants, Explosives, Pyrotechnics*, **2012**, *37*, 489–497.
[6] M. H. Keshavarz, *Propellants, Explosives, Pyrotechnics*, **2008**, *33*, 448–453.
[7] M. Jafari, M. Kamalvand, M. H. Keshavarz, A. Zamani, H. Fazeli, *Indian J. Engineering and Mater. Sci.*, **2015**, *22*, 701–706.
[8] S. M. Kaye, *Encyclopedia of Explosives and Related Items*, *vol. 8*, US Army Research and Development Command, TACOM, Picatinny Arsenal, USA, **1978**.
[9] L. R. Rothstein, R. Petersen, *Propellants and Explosives,* **1979**, *4*, 56–60.
[10] J. Bebie, *Manual of Explosives, Military Pyrotechnics and Chemical Warfare Agents, Composition, Properties, Uses*, MacMillan Co., **1943**.
[11] P. W. Cooper, *Explosives Engineering*, Wiley, **1996**.
[12] B. Nazari, M. H. Keshavarz, M. Hamadanian, S. Mosavi, A. R. Ghaedsharafi, H. R. Pouretedal, *Fluid Phase Equilibria,* **2016**, *408*, 248–258.

Ethyltetryl

Name [German, acronym]: *N*-Ethyl-*N*,2,4,6-tetranitroaniline, ethyltetryl, (2,4,6- trinitrophenylethylnitramine) ethane, *N*-ethyl-*N*-nitro-2,4,6-trinitroaniline, ethylpicrylnitroamine, 2,4,6-trinitrophenylethylnitramine, [*N*-nitro-*N*-äthyl-2,4,6-trinitroanilin]

Main (potential) use: Component of energetic pourable mixtures[1]

Structural formula:



	Ethyltetryl
Formula	$C_8H_7N_5O_8$
Molecular mass [g mol^{-1}]	301.17
Appearance at RT	Green-yellow crystals[1], crystalline solid[11]
IS [J]	5 Nm[1], FI = 92% PA[6], 48% detonations with 2 kg mass falling 2.5 m[6]
FS [N]	>353[1]
N [%]	23.25
Ω(CO_2) [%]	−61.1
$T_{m.p.}$ [°C]	95.8[1, 2], 95–96[6, 10], 96[9, 11], 94 (recryst. twice from nitric acid and once from EtOH)[9]
$T_{dec.}$ [°C]	
ρ [g cm^{-3}]	1.63[1], 1.713 ± 0.06 (@ 293.15 K)[3], sp. gr. = 1.644 (@ 10°)[6]
Heat of formation	0 ± 1.0 kcal/mol (ΔH_f^{298})[2], −7.70 kcal/mol ($\Delta_f H$)[2], −59.8 kJ/kg (enthalpy of form.)[1], 18.0 kJ/mol (enthalpy of form., exptl.)[13], −34.0 kJ/mol (enthalpy of form., calcd., emp.)[13], −55.1 kJ/mol (enthalpy of form., calcd., S-D method)[13]
Heat of combustion	994 ± 1.0 kcal/mol (ΔQ_c, isochore)[2], 990.41 kcal/mol (ΔQ_c)[2]

	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]	4,132 (calcd., K-J)[4]		4,058 [H_2O (l)][1] 3,930 [H_2O (g)][1]
T_{ex} [K]			
$p_{C\text{-}J}$ [GPa]	22.9		
VoD [m s^{-1}]	7,482 (@ TMD)		6,200 (@ sp. gr. = 1.10)[6]
V_0 [L kg^{-1}]	674		874[1, 5]

Trauzl test [cm^3, % TNT]	325 cm^3 (10 g sample)[1], 114% TNT[7], 325 cm^3[12]
Ballistic mortar test	111% TNT[7]
Fugacity	104% PA[11]
ΔH_{melt} [kcal/mol]	5.62 ± 0.11[2]
$C_p{}^{298}$ [cal mol^{-1}K^{-1}]	79.4[2], 113.0 ± 1.4 (C_p liq.)[2]

	Ethyltetryl[8]
Chemical formula	$C_8H_7N_5O_8$
Molecular weight [g mol^{-1}]	301.19
Crystal system	Monoclinic
Space group	$P2_1/c$ (no. 14)
a [Å]	15.020(10)
b [Å]	7.5040(10)
c [Å]	10.6610(10)
α [°]	90
β [°]	93.160(10)
γ [°]	90
V [Å^3]	1,202.3(2)
Z	4
ρ_{calc} [g cm^{-3}]	1.664
T [K]	293

[1] R. Meyer, J. Köhler, A. Homburg, *Explosives*, 7th edn., Wiley-VCH, Weinheim, **2016**, pp. 130–131.
[2] G. Krien, H. H. Licht, J. Zierath, *Thermochimica Acta,* **1973**, *6*, 465–472.
[3] Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© **1994–2017** ACD/Labs).
[4] M. H. Keshavarz, M. Ghorbanifaraz, H. Rahimi, M. Rahmani, *Propellants, Explosives, Pyrotechnics,* **2011**, *36*, 424–429.
[5] M. Jafari, M. Kamalvand, M. H. Keshavarz, A. Zamani, H. Fazeli, *Indian J. Engineering and Mater. Sci.,* **2015**, *22*, 701–706.
[6] B. T. Fedoroff, O. E. Sheffield, *Encyclopedia of Explosives and Related Items*, *vol. 6*, US Army Research and Development Command, TACOM, Picatinny Arsenal, USA, **1974**.
[7] 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**.
[8] Z. G. Aliev, A. V. Shastin, S. M. Aldoshin, *Zh. Strukt. Khim.*, **2015**, *56*, 1203; *Russ. J. Struct. Chem. (Engl. Transl.)*, **2015**, *56*.
[9] T. L. Davis, *The Chemistry of Powder and Explosives*, *vol. 1*, **1941**, John Wiley and Sons Inc., New York, p. 183.
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[12] M. Jafari, M. Kamalvand, M. H. Keshavarz, S. Farrashi, *ZAAC*, **2015**, *641*, 2446–2451.
[13] B. Nazari, M. H. Keshavarz, M. Hamadanian, S. Mosavi, A. R. Ghaedsharafi, H. R. Pouretedal, *Fluid Phase Equilibria,* **2016**, *408*, 248–258.

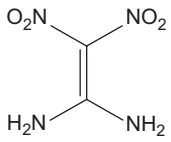
F

FOX-7

Name [German, acronym]: 1,1-Diamino-2,2-dinitroethene, 2,2-dinitroethene-1,1-diamine [FOX-7, DADNE]

Main (potential) use: Secondary (high) explosive, thermally stable explosive[36], in explosive compositions which need to have low sensitivity to external stimuli[41], possible new explosive ingredient in insensitive munition (IM) compliant explosive compositions[49]

Structural formula:



	FOX-7
Formula	$C_2H_4N_4O_4$
Molecular mass [g mol^{-1}]	148.08
Appearance at room temperature (RT)	Yellow solid[24]
IS [J]	25 (<100 µm), 15–40 Nm[1], 25[2], 120 cm with 2.5 kg hammer[6], >25 Nm[9], Rotter FoI = 110–140 (powder)[13], 63–79 cm (powder, US drop hammer)[13], 11.5 ($DADNE_{coarse\text{-}grain}$, H = 23 cm, 5 kg hammer, highest drop height at which no reaction observed)[16], 14 ($DADNE_{coarse\text{-}grain}$/$DADNE_{fine\text{-}grain}$, 70/30, H = 28 cm, 5 kg hammer, highest drop height at which no reaction observed)[16], 26.5 ($DADNE_{vit}$ (DADNE phlegmatized by Viton), H = 53 cm, 5 kg hammer, highest drop height at which no reaction observed)[16], H_{50} = 72 cm[17], 24.7 Nm ((H_{50}Wg)$^{-1}$)[18], H_{50} = 126 cm (30.9 J)[19], 126 cm (2 kg mass, BAM)[23, 24], 20 Nm (ball milled)[25], 20 Nm (Fox-7 processed by PCA)[25], 79 cm (highest drop height without reaction, recryst. Fox-7, 250–355 µ,)[26], 63 cm (highest drop height without reaction, recryst. Fox-7, <70 µm)[26], Rotter impact F of I = 100[27], Rotter impact FoI = 110 (Fox-7/PE-wax (98.75/1.25))[27], 15 Nm (large particle)[29], 35 Nm (small particle)[29], 15–30 (BAM)[30], 28% probability of explosion @ 25 cm (10 kg mass, 50 mg powder, WL-1 apparatus)[31], H_0 = 23 cm (11.3 J, highest drop height at which no reaction was observed, 5 kg hammer)[32], H_{50} = 35.2 cm (17.3 J, 5 kg hammer)[32], 15.5 (crystals 250–355 µm, 2 kg hammer)[32], 12.4

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<table>
<tr>
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<td>(crystals <70 µm, 2 kg hammer)[32], 24.7 (50% probability, 2 kg drop weight, crystalline Fox-7)[32], 31.2 (50% probability, 2 kg drop weight, recrystallized Fox-7)[32], Ed_{min} = 20 (BAM, 5 kg mass, RT)[33], 15 Nm[34], 126 cm (2 kg mass, BAM)[35], 6% (10 kg, 25 cm)[42], $H_{50\%}$ = 89.1 cm (5 kg mass)[42], FoI = 100 (Bofors nonrecryst., Rotter impact)[42], FoI = 100 (Bofors, recryst., Rotter impact)[42], 110–140 (DSTO, nonrecryst., Rotter impact)[42], 79 cm (highest drop height at which no reaction occurs, 2 kg mass, recryst. Fox-7, 250–355 µm)[42], 63 cm (highest drop height at which no reaction occurs, 2 kg mass, recryst. Fox-7, <70 µm)[42], A_{d1} = 16%, A_{d2} = 72%, LL = 1.2 m, $A_{50\,d1}$ = 5.8 m, $A_{50\,d2}$ = 1.6[47]

IS (5 kg mass, BAM, H = highest drop height at which no reaction was observed, E_i = impact energy at this drop height)[41]:

<table>
<tr><td></td><td>Fox-7_c</td><td>Fox-7_f</td><td>Fox-7</td></tr>
<tr><td></td><td>100% coarse Fox-7, particle size = 250–500 µm</td><td>100% fine Fox-7, particle size = 5–11 µm</td><td>30% Fox-$_f$, 70% Fox-$_c$, mixture of fine and coarse Fox-7</td></tr>
<tr><td>H (cm)</td><td>23</td><td>39</td><td>28</td></tr>
<tr><td>E_i (J)</td><td>11.5</td><td>19.5</td><td>14</td></tr>
</table>

Solvents used affect the IS of Fox-7[42]:

<table>
<tr><td>Property</td><td>NMP/H_2O</td><td>NMP/H_2O + antisolvent</td></tr>
<tr><td>Mean particle size (µm)</td><td>213</td><td>273</td></tr>
<tr><td>Span (90/10)</td><td>1.445</td><td>0.506</td></tr>
<tr><td>IS (Nm)</td><td>25</td><td>35</td></tr>
</table>

4% (recryst. from DMSO/H_2O)[48], 4% (recryst. from DMF/H_2O)[48], 8% (recryst. from cyclohexanone)[48], 110–140 (Rotter FoI, uncrystallized, average gas evolution = 5.7 mL cf. Rotter FoI = 80 for RDX with 11.9 mL average gas evolution)[49], 126–159 cm (recryst., 2 kg mass, BAM)[49]</td>
</tr>
<tr>
<td>FS [N]</td>
<td>>360 (<100 µm), 216[1], >350[2], >360[9] , $P_{fr.LL}$ = 330 MPa[12, 47], $P_{fr50\%}$ = 450 MPa[12, 47], >350 (Julius–Petri)[23, 24], 144 (ball milled)[25], 288 (Fox-7 processed by PCA)[25], 240 (BAM)[27], 216 (Fox-7/PE-wax (98.75/1.25))[27], 216 (large particle)[29], 192 (small particle)[29], 160–240 (BAM)[30], 40% probability of explosion (WM-1 apparatus)[31], >353 (Julius-Peters)[32], G_{min} = 360 (BAM Julius-Peters, max. level with six consec. negative runs)[32], 252[34], 350[35], >353 (Fox-7_c, coarse particles, 250–500 µm)[41], >353 (Fox-7_f, fine particles, 5–11 µm)[41], >353 (Fox-7, 30% fine particles, 70% coarse particles)[41], 10% (3.92 MPa, 90°)[42], 240 (Bofors nonrecryst., BAM)[42], 240 (Bofors, recryst., BAM)[42], 166–288 (DSTO, nonrecryst., BAM)[42], 4% (recryst. from DMSO/H_2O)[48], 4% (recryst. from DMF/H_2O)[48], 48% (recryst. from cyclohexanone)[48], 168–288 (unrecrystallized, Julius-Peters BAM)[49], >350 (purified, Julius-Petri apparatus)[49]</td>
</tr>
</table>

<table>
<tr><td></td><td>Solvents used affect the FS of Fox-7[42]:

<table><tr><td>Property</td><td>NMP/H_2O</td><td>NMP/H_2O + antisolvent</td></tr><tr><td>Mean particle size (µm)</td><td>213</td><td>273</td></tr><tr><td>Span (90/10)</td><td>1.445</td><td>0.506</td></tr><tr><td>FS (N)</td><td>240</td><td>192</td></tr></table></td></tr>
<tr><td>ESD [J]</td><td>1.0 (<100 µm), ~4.5[2], 4.5[27], V_{50} = 13.13 kV (JGY apparatus)[31], E_{50} = 2.642 (JGY apparatus)[31], energy in capacitors = 625 mJ, spark duration = short[39], ignition @ 4.5, no ignition @ 0.45 (Bofors nonrecryst.)[42], ignition @ 4.5, no ignition @ 0.45 (Bofors, recryst.)[42], ignition @ 4.5, no ignition @ 0.45 (DSTO, non-recryst.)[42], ignition @ 4.5 but not @ 0.45[49]</td></tr>
<tr><td>N [%]</td><td>37.84</td></tr>
<tr><td>$\Omega(CO_2)$ [%]</td><td>−21.61</td></tr>
<tr><td>$T_{m.p.}$ [°C]</td><td>Deflagration above 240 °C[1], 205[43], no mpt. observed in DSC @ 5 °C/min[49]</td></tr>
<tr><td>$T_{phase\ transition}$ [°C]</td><td>DTA (@ 2 °C/min), endotherm peaks[10]:

<table><tr><td>Fox-7 sample recryst. From</td><td>T (°C) (onset)</td><td>T (°C) (onset)</td></tr><tr><td>H_2O, mix of crystals</td><td>113</td><td>178</td></tr><tr><td>Acetone, mix of crystals</td><td>115</td><td>158</td></tr><tr><td>Acetone, tetrahedral prisms</td><td>112</td><td>160</td></tr><tr><td>H_2O–acetone mix, tetrahedral prisms</td><td>115</td><td>158</td></tr><tr><td>H_2O–acetone mix, trimetric crystals</td><td>114</td><td>155</td></tr></table>
Particle size versus $T_{dec.}$[24]: 116 (endo), 158 (endo) (DSC, single crystal, 1.5 mg sample)[24, 37], 119 (endo, peak max.) (DSC, very fine powder, 1.5 mg sample)[24], phase change <100 °C suggested based on X-ray powder diffraction[37]

Data from[24]:

α-Fox-7 $\underset{\text{(i)}}{\overset{\sim 80\ ^\circ C}{\rightleftharpoons}}$ β-Fox-7 $\underset{\text{(ii)}}{\overset{115\ ^\circ C}{\rightleftharpoons}}$ γ-Fox-7 $\overset{156\ ^\circ C}{\rightleftharpoons}$ δ-Fox-7 $\overset{225\ ^\circ C}{\rightleftharpoons}$

(i) Particle size strongly affects the T at which this phase transitions occurs at, that is, fine particles @ ~78 °C, larger particle @ ~95 °C, phase transition requires 3 h and the time is independent of the particle size. Fully reversible phase transition[24]</td></tr>
</table>

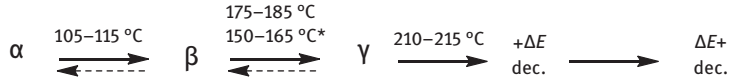
(ii) Phase transition is not influenced by particle size. But particle size influences time required for the phase transition, that is, fine particles require 10 h, larger particles require 14 h, very slow kinetically for reverse and takes up to 4 weeks for γ-Fox-7 to revert back to α-Fox-7[24]

α-phase occurs @ ambient *T*[36], reversible α- → β-phase transition @ ~113 °C[36], phase transition @ ~160 or ~170[36]

Fox-7 crystallizes in α-phase (stable up to 112 °C) from H_2O, acetone or DMF[36], crystals contain 0.1–1% solvent which is released @ phase transition[36] samples recryst. from H_2O, acetone or DMF undergo β- → γ- @ 150–170 °C; or @ 175–185 °C for very fine crystalline sample obtained by pouring hot DMF soln. into H_2O and which contains no solvent inclusion[36]

~105–115 (endo), ~175–185 °C (endo)[38], one polymorphous modification of Fox-7 is stable at *T* > 215 °C but the transition occurs parallel with some dec. (DADNE-T)[38], first endo peak @ 105–115 °C regardless of solvent used for recryst.[38], onset of second endo peak depends on solvent used for recryst.[38]

Assumed polymorphous transitions in Fox-7[38]:



* = Crystallized Fox-7

Phase transitions as reported by *Bemm* and *Eriksson* cited in[37]:

Phase	Formation *T* (°C)	Comments
α-		Monoclinic, $P2_1/n$, $\rho = 1.91$ g cm^{-3}
β-	~ 85	Orthorhombic, 4.3% vol. increase from α-, α-→ β- Second order monoclinic → Orthorhombic transition, occurs over 75–95 °C *T* interval but is not visible by DSC
γ-	~ 115	formed directly from α- @ high heating rates
δ-	~ 155	

Uncertainty over whether broad feature in DSC ~ 150 °C is baseline or δ- → γ- transition[37], reversion @ 75 °C on cooling rate of 3 °C/min (or @ 50 °C with cooling rate of 30 °C/min) is direct transformation from δ- → α- phase[37], ~114 °C (β- → γ-) and ~159 °C (β- → γ-) both detected @ ambient pressure and @ 8.85 MPa (modified heat flow calorimeter (HFC)) Fig. 8[37]

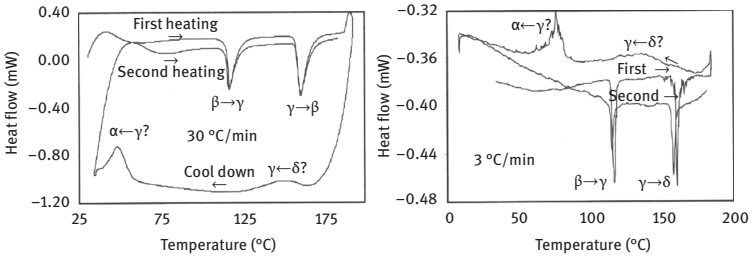


Fig. 8: Cyclic heating and cooling of FOX-7 at 30 °C/min (left) and 3 °C/min (right)[37].

Summary of phase transition data @ various heating rates (DSC)[37]:

Heating rate (°C/min)	β- → γ-		γ- → δ-	
	T_p (°C)	ΔH (J/g)	T_p (°C)	ΔH (J/g)
0.1	114.5	25.3	158.5	15.0
0.35	114.9	21.3	158.9	14.6
1.0	115.8	18.7	160.4	16.8
3.0	118.1	21.9	164.7	21.0
10	119.7	21.5	163.8	18.7
30	122.3	20.7	165.3	20.0

387 K (onset), 388 K (peak max.) α- → β- (DSC)[42], ~430 K (onset), ~435 K (peak max.) β- → γ- (DSC)[42], γ- stable up to 504 K[42], 390 K α- → β-[42], 440 K β- → γ-[42]

Phase transitions not altered by solvent crystals are obtained from (solvents used = DMF/H_2O, DMSO/H_2O and NMP/H_2O): α- is crystal phase @ RT[46], α- → β- @ 120 °C[46], β- → γ- @ 185 °C[46]

α-Fox-7 obtained on recryst. from DMSO/H_2O, glacial acetic acid, cyclohexanone, acetonitrile and DMF/H_2O[48], 112–115 (minor endo), 165–172 (minor endo) (DSC @ 5 °C/min)[49]

$T_{dec.}$ [°C]

219 (DSC @ 5 °C/min)[10], 215 (dec. onset)[20], 283.15 (onset), 283.83 (peak max.) (DSC)[35]

DTA (@ 2 °C/min), exotherm peaks[10]:

Fox-7 sample recryst. from	T (°C) (onset) dec. stage 1	T (°C) (onset) dec. stage 2
H_2O, mix of crystals	207	277
Acetone, mix of crystals	213	279
Acetone, tetrahedral prisms	226	273
H_2O-acetone mix, tetrahedral prisms	213	278
H_2O-acetone mix, trimetric crystals	213	279

T corresponding to max. rate of decomposition[16, 41]:

Heating rate (°C/min)	DADNE		DADNE Phlegmatized by Viton	
	First stage (°C)	Second stage (°C)	First stage (°C)	Second stage (°C)
1	215.9	274.0	215.7	276.0
2	220.4	278.3	219.8	278.3
3	222.7	277.0	223.3	277.7
4	224.9	275.3	224.8	278.3
5	227.4	274.4	228.1	276.5

Particle size versus $T_{dec.}$[24]: ~235 (exo, DSC, single crystal, 1.5 mg sample)[24], ~220 (exo, peak max.), ~258 (exo, peak max.), ~280 (exo peak max.) (DSC, very fine powder, 1.5 mg sample)[24]

Two step dec.: @ ~215 (peak max., @ 0.5 K/min, ~40% mass loss), @ 280 (peak max., @ 0.5 K/min, ~45% mass loss)[36]

TGA/DTA (@ 2 °C/min up to 230 °C, open 100 µm Pt pans, He flow of 50 cm^3/min) causes complete dec. only in the Fox-7 sample obtained by slow-cooling crystallization from DMF; other samples showed mass loss of ~30% regardless of crystallization conditions[36], only partial dec. or on heating to 230 °C for fine Fox-7 crystals precipitated from hot Fox-7 soln. in DMF after pouring into water, crystals contain no solvent, dec. peak max. occurs @ ~10 °C lower than 230 °C[36]

Fox-7 recryst. from H_2O and heated @ 160 °C for 10 h shows similar dec. profile as sample without preheating @ 160 °C[36], onset of first exo peak depends on solvent used for recryst. (DTA)[38], onset of second exo peak @ ~270–280 °C regardless of solvent used for recryst. (DTA)[38], shapes, areas and observed dec. *T* of the two dec. peaks @ ~235 °C and ~280 °C vary with different batches and sources of the sample – sometimes, these two peaks are merged into one (DSC)[37]

Summary of thermal dec. data @ different heating rates (DSC unless otherwise indicated)[37]:

Heating rate (°C/min)	First exotherm		Second exotherm		Total	First DTG	Second DTG
	T_p (°C)	$-\Delta H$ (kJ/g)	T_p (°C)	$-\Delta H$ (kJ/g)	$-\Delta H$ (kJ/g)	T_p (°C)	T_p (°C)
0.10	202.3	1.98	261.7	0.61	2.59	201	260
0.35	210.6	1.20	271.7	0.99	2.19	209	269
1.0	217.3	1.20	278.6	1.14	2.34	217	277
3.0	226.2	0.85	277.2	0.96	1.82	–	–
10	238.3	0.52	274.0	1.40	1.92	–	–
30	249.5	0.52	278.8	1.39	1.91	–	–

233 (one sharp exo peak, modified HFC, @ 0.07 MPa (ambient pressure))[37], 239 and 244 (two exo peaks , modified HFC, @ 8.85 MPa (ambient pressure))[37], two major exothermic peaks @ 214–238 °C and 250–276 °C which occassionally merge into almost one peak (two-stage thermal dec., DSC @ 5 °C/min)[49]

ρ [g cm^{-3}]	1.8934 (@ 298 K), 1.850 (gas pycnometer), 1.89 (α-polymorph)[9], 1.80 (β-polymorph)[9], 1.885[17, 20, 42], 1.878 (X-ray)[24], 1.885 (powder diffraction)[24, 49], 1.907 (@ 298 K)[30], 1.878 (crystal density)[49], 1.86–1.87 (He pycnometry)[49]
Heat of formation	−134 kJ/mol ($\Delta_f H$)[4], −119 kJ/mol ($\Delta_f H$)[1], −32 kcal/mol ($\Delta_f H$ (s))[17, 42], +130.0 kJ/mol (enthalpy of form.)[20], −209.0 kcal/kg (enthalpy of form.)[21], −134 kJ/mol ($\Delta_f H$)[30], −32 kcal/mol (exptl. bomb calorimetry)[49]

	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]	4,958	1,200 cal/g (calcd. K-J)[4] 921.1 cal/g (calcd., K-W)[4]	4,442 J/g [H_2O (L)][9] 4,091 J/g [H_2O (g)][9]

		921.1 cal/g (calcd., mod. K-W)[4] 1.20 kcal/g (Q_{max}, calcd.)[17] 4,860[20] 1,064 kcal/kg (@ 1.810 g cm^{-3}, calcd.) [H_2O vapor][21] 724.4 kJ/mol ($\Delta_{ex}H$)[30] 4.892 kJ g^{-1} ($\Delta_{ex}H$)[30] 4,774 J/g (calcd., BKWC, CHEETAH)[32] 4,849 J/g (calcd., BKWR, CHEETAH)[32]	1,090 kcal kg^{-1} [H_2O (g)][8] 1,090 kcal/kg (@ 1.810 g cm^{-3}) [H_2O vapor][21] 4,860 ± 60 J/g (heat of detonation, 5 dm^3 calorimetric bomb, filled with Ar @ 2 MPa, 20 g charge, detonated by electric fuse)[32] 1,090 kcal/kg (@ 1.81 g cm^{-3}, Q_{exp})[40]
T_{ex} [K]	3,318	2,917 (@ 1.885 g cm^{-3}, $\Delta H_f = -133.9$ kJ/mol, calcd., JAGUAR)[45]	
$p_{C\text{-}J}$ [kbar]	335	37.08 GPa (@ 1.885 g cm^{-3}, calcd., CHEETAH 2.0)[3] 340 (calcd., K-J)[4] 340 (calcd., K-W)[4] 340 (calcd., mod. K-W)[4] 34.0 GPa (@ 1.885 g cm^{-3}; $\Delta_f H = -53.4$ kJ mol^{-1}, calcd. CHEETAH 1998)[15] 338 (@ 1.885 g cm^{-3}, calcd.)[17] 29.34 (@ 1.780 g cm^{-3}, calcd., CHEETAH)[22] 34.0 GPa (@ 1.885 g cm^{-3}, $\Delta H°_f = -53.4$ kJ/mol, calcd., CHEETAH)[33]	29.2 GPa (@ 1.780 g cm^{-3}, calcd. from eqn. based on water test values)[22] 28.4 GPa (@ 1.780 g cm^{-3}, calcd. from eqn. based on water test values)[22] 28.4 (@ 1.780 g cm^{-3}, cylinder test no. 3)[22]

		28.4 GPa (@ 1.780 g cm^{-3})[42] 35.0 GPa (@ 1.885 g cm^{-3}, $\Delta H_f = -133.9$ kJ/mol, calcd., JAGUAR)[45]	
VoD [m s^{-1}]	8,877 (@ TMD)	9,126 (@ 1.885 g cm^{-3}, calcd., CHEETAH 2.0)[3] 8,630 (@ 1.89 g cm^{-3}, calcd., K-J)[4] 8,630 (@ 1.89 g cm^{-3}, calcd., K-W)[4] 8,630 (@ 1.89 g cm^{-3}, calcd., mod. K-W)[4] 8,683 (@ 1.78 g cm^{-3}, calcd. BKWR)[14] 8,558 (@ 1.78 g cm^{-3}, calcd. BKWS)[14] 8,870 (@ 1.885 g cm^{-3}; $\Delta_f H = -53.4$ kJ mol^{-1}, calcd. CHEETAH 1998)[15] 8,610 (@ 1.885 g cm^{-3}, calcd.)[17] 8,453 (@ 1.780 g cm^{-3}, calcd. CHEETAH)[22] 8,870 (@ 1.88 g cm^{-3})[23] 8,453 (@ 1.780 g cm^{-3}, calcd., BKWC, CHEETAH)[32] 8,451 (@ 1.780 g cm^{-3}, calcd., BKWS, CHEETAH)[32] 8,870 (@ 1.885 g cm^{-3}, $\Delta H^{o}_f = -53.4$ kJ/mol, calcd., CHEETAH)[33]	8,869 (@ 1.89 g cm^{-3})[4] 8,335 (@ 1.76 g cm^{-3})[7] 8,450 (@ 1.780 g cm^{-3}, water test)[22] 8,375 (@ 1.780 g cm^{-3}, water test)[22] 8,325 (@ 1.780 g cm^{-3}, cylinder test no. 3)[22] 8,290 (@ 1.780, Cu cylinder test, short-circuit sensors, 300 mm long tube, 25 mm internal diameter, 2.5 mm wall thickness)[32] 8,300 (@ 1.780, Cu cylinder test, short-circuit sensors, 300 mm long tube, 25 mm internal diameter, 2.5 mm wall thickness)[32] 8,325 ± 80 (@ 1.780 g cm^{-3})[32] 8,047 (@ 1.696 g cm^{-3})[42]

		8,226 (@ 1.756 g cm^{-3}, calcd., CHEETAH, BKWC)[42] 8,800 (@ 1.885 g cm^{-3}, ΔH_f = –133.9 kJ/mol, calcd., JAGUAR)[45]	8.335 ± 0.025 mm/µs (@ 1.756 g cm^{-3}, FOX-7 containing 1.5 wt.% wax, 300 mm length, 30.2 mm diameter, 2.52 mm shell thickness)[42] 8,325 ± 50 (based on cylinder test data)[42]
V_0 [L kg^{-1}]	781		779 [5]

Critical diameter [cm]	Critical detonation diameter d_{c0} [mm] and specific surface area, S_g [cm^2 g^{-1}] @ rel. high density (0.98–0.995)[20]: S_g (cm^2 g^{-1}) | d_{c0} (mm) | S_g (cm^2 g^{-1}) | d_{c0} (mm) 650 | 2.85 | 2,900 | 1.00 1,500 | 1.90 | 8,000 | 0.75 d_{c0} (mm) @ mean crystal size (µm)[20]: 0.55 @ 3, 1.05 @ 10, 1.60 @ 20[20]
Critical pressure of initiation of explosive [GPa]	P_{cr} = 1.05[40], σ_{ult} = 75 MPa[40]
Koenen test	Type F reaction (explosion) @ 6 mm nozzle diameter[24, 49], 6 mm/type F (tube fragmented into 3 or more large pieces, which in some cases may be connected to each other by a narrow strip)[30]
Gap test	Gap = 56 mm, gap = 57 mm (fine grain)[16], gap = 68 mm, gap = 69 mm (coarse grain)[16], gap = 57 mm, gap = 58 mm (Fox-7 phlegmatized by Viton)[16]
LSGT [cm]	P_{50} = 4–6.5 GPa (NOL-LSGT, shock sensitivity decreases with increasing particle size)[30]
SSGT [cm]	18.5 mm (Fox-7/PTFE, 90/10, ρ = 1.84 g cm^{-3}, BICT-SSGT)[44], implies low sensitivity to shock stimuli[49], 6.22 mm (recryst., NOL SSGT)[49]
5 s explosion T [°C] Ignition T [°C]	285[42], 274.0 (crystals from DMF/H_2O)[46], 274.0 (crystals from DMSO/H_2O)[46], 269.0 (crystals from NMP/H_2O)[46] 215 (Wood's metal bath)[24, 49], 226[27], 236 (Fox-7/PE-wax (98.75/1.25))[27], 217 (Bofors, nonrecryst.)[42], 226 (DSTO, non-recryst.)[42], 225 (heating rate 5 °C/min)[49]

<table>
<tr><td>Thermal stability</td><td>DTA: Fox-7 shows two exothermic peaks @ ~210 °C (onset) and ~275 °C (onset), 30–35% mass loss after completion of first exothermic process[38], total mass loss = 83% in He (two-step dec. process, TG-DTA-FTIR-MS @ 5 °C/min, also minor mass loss @ 161 °C assumed due to impurities in sample)[37], total mass loss = 93% in air (two-step dec. process, TG-DTA-FTIR-MS @ 5 °C/min, also minor mass loss @ 205 °C assumed due to impurities in sample)[37]</td></tr>
<tr><td>Vacuum stability test [cm^3/h]</td><td>0.14 mL/5 g @ 100 °C, 48 h[42], 0.28 mL/g @ 100 °C, 48 h (Bofors, nonrecryst.)[42], <0.1 mL/g @ 100 °C, 48 h (DSTO, nonrecryst.)[42, 49]</td></tr>
<tr><td>Vapor pressure [atm. @ °C]</td><td>1.04×10^{-3} mm Hg (solid)[43]</td></tr>
<tr><td>Solubility [g/mL]</td><td>~1.6 g / 100 g H_2O @ 100 °C[32], NMP (N-methyl-2-pyrrolidone) is one of the best solvents for Fox-7[32], Fox-7 can be recrystallized from H_2O, acetone or DMF, however, Fox-7 recrystallized as a hot DMF soln. poured into H_2O shows a 10 °C lower $T_{dec.}$ than Fox-7 recryst. from H_2O or acetone[36], 1.00×10^6 mg/L in H_2O[43], poorly soluble in common organic solvents and water[49], readily dissolves in aprotic solvent, for example, DMSO, DMF and NMP[49], can be recryst. from dil. hydrochloric acid, γ-butyrolactone or water[49], can be recryst. by dissolving in hot DMF or NMP (@ 70 °C) and then adding 4–5 equivalents of hot EtOH, MeOH or water to precipitate Fox-7[49]

solubility in H_2O (conc. of Fox-7 (% wt.) @ T (°C)): ~0.02 @ 20 °C, ~0.1 @ 40 °C, ~0.2 @ 60 °C, ~0.55 @ 80 °C, ~1.6 @ 100 °C[36], saturated aq. soln. @ 100 °C contains ~1.6% Fox-7[36]</td></tr>
<tr><td>Compatibility</td><td>Thermal stability and compatibility of Fox-7 with different polymers[24]:

<table>
<tr><th>Polymer or plasticizer</th><th>E_b (J/g)</th><th>C_{ab} (J/g)</th><th>Polymer or plasticizer</th><th>E_b (J/g)</th><th>C_{ab} (J/g)</th></tr>
<tr><td>CAB (BF900)</td><td>0.38</td><td>–0,38</td><td>Krasol LBH</td><td>0.24</td><td>0.13</td></tr>
<tr><td>ESTANE</td><td>0.27</td><td>–0.26</td><td>VITON</td><td>0.10</td><td>0.03</td></tr>
<tr><td>GAP</td><td>2.57</td><td>–0.44</td><td>Butyl-NENA</td><td>1.07</td><td>0.16</td></tr>
<tr><td>HTPB (R-45HT)</td><td>1.89</td><td>3.89</td><td>K-10</td><td>0.41</td><td>0.44</td></tr>
</table>

Excellent compatibility with typical components of explosive formulations and propellants[36], Fox-7 should not be recrystallized form a hot DMF solution by pouring into water since it results in a lowering of the dec. T by ~10 °C cf. Fox-7 recrystallized from H_2O or acetone[36], compatibility assessed by heat flows in microcalorimeter[49]: excellent compatibility with GAP, HMDI, Butyl-NENA and K-10[49], very low compatibility with HTPB[49], 1:1 mixture of TNT and Fox-7 showed same stability as individual components under same conditions (vacuum thermal stability, 100 °C, 48 h)[49]</td></tr>
<tr><td>pK_a</td><td>10.6[23]</td></tr>
</table>

<table>
<tr><td>ARC (accelerated rate calorimetry) [°C]</td><td>Runaway reaction @ ~230[24], 210 (onset) (ϕ = 8.66)[30], 221 ± 2 (reaction onset T), 230 ± 1 (runaway T)[49]

T range 150–400 °C, onset and runaway T @ 150 °C and 180 °C[24]:

<table>
<tr><td>Fox-7</td><td colspan="2">Wait time 5 min</td><td colspan="2">Wait time 10 min</td><td colspan="2">wait time 15 min</td></tr>
<tr><td>Start T (°C)</td><td>150</td><td>180</td><td>150</td><td>180</td><td>150</td><td>180</td></tr>
<tr><td>Onset T (°C)</td><td>222</td><td>222</td><td>222</td><td>219</td><td>223</td><td>223</td></tr>
<tr><td>Runaway T (°C)</td><td>230</td><td>231</td><td>230</td><td>229</td><td>230</td><td>230</td></tr>
</table>

Detectable heat release after ~100 h, sample runaway @ ~233 °C (isothermal, 200 mg sample in Ar, @ 200 °C, 96 h, closed system)[37], sample runaway after 41 h (isothermal, 200 °C, 1 g sample in Ar)[37], sample runaway after 28 h (isothermal, 210 °C, 1 g sample in Ar)[37]</td></tr>
<tr><td>Average particle size [µm]</td><td>25 (scale-up batches, granular)[24]</td></tr>
<tr><td>Heat capacity, C_p [J g^{-1} K^{-1}]</td><td>1.455[30]</td></tr>
<tr><td>Specific heat [J mol^{-1} K^{-1}]</td><td>Exptl. values[42]: 266.6 @ 283 K[42], 272.0 @ 288 K[42], 277.1 @ 293 K[42], 281.9 @ 298 K[42], 286.4 @ 303 K[42], 290.7 @ 308 K[42], 294.7 @ 313 K[42], 298.4 @ 318 K[42], 301.8 @ 323 K[42], 305.0 @ 328 K[42], 307.9 @ 333 K[42], 310.5 @ 338 K[42], 312.8 @ 343 K[42], 314.9 @ 348 K[42], 316.7 @ 353 K[42]</td></tr>
<tr><td>ODTX [°C/s]</td><td>260/15 (Fox-7/Viton® A, 95:5)[30]</td></tr>
<tr><td>Gurney energy [kJ/kg]</td><td>3,568 (@ 1.780 g cm^{-3}, cylinder test, impulse X-ray apparatus, 300 mm long tube, 25 mm internal diameter, 2.5 mm wall thickness)[32], 3,672 (@ 1.780 g cm^{-3}, cylinder test, impulse X-ray apparatus, 300 mm long tube, 25 mm internal diameter, 2.5 mm wall thickness)[32], 3,540 ± 100[42]</td></tr>
<tr><td>Gurney velocity [m/s]</td><td>2,671 (@ 1.780 g cm^{-3}, cylinder test, impulse X-ray apparatus, 300 mm long tube, 25 mm internal diameter, 2.5 mm wall thickness)[32], 2,710 (@ 1.780 g cm^{-3}, cylinder test, impulse X-ray apparatus, 300 mm long tube, 25 mm internal diameter, 2.5 mm wall thickness)[32], 2,660 ± 40[42]</td></tr>
<tr><td>Activation energy to thermal dec. [kcal/mol]</td><td>~50–90 in T range ~200–250 °C[38], 238.3 kJ/mol (first exotherm, Kissinger's method, DSC)[37], 322.4 kJ/mol (second exotherm, Kissinger's method, DSC)[37], ΔH = –1.65 kJ g^{-1} (one sharp exo peak @ 233 °C, modified HFC, @ 0.07 MPa (ambient pressure)[37], ΔH = –2.10 ± 0.06 kJ/g (@ ~230 °C, DSC shows two exo peaks)[37], ΔH = –3.04 ± 0.06 kJ/g @ 239 and 244 °C (two exo peaks, modified HFC, @ 8.85 MPa (ambient pressure)[37], 191 ± 4 kJ/mol (initial activation energy of dec., isothermal TG-DTA-FTIR-MS)[37]</td></tr>
<tr><td>Log K_{ow}</td><td>–2.86 (SMILES, predicted, EPI)[42], –2.86 (SMILES and MP, predicted, EPI)[42], K_{ow} = 0.0014 l/kg[43]</td></tr>
</table>

K_{oc}	30.6 L/kg[43]
Half life in soil [days]	15.8[43]
Half life in water [days]	15.8[43]
Beckford fuze	Ignition (Bofors, nonrecryst.)[42], fails to ignite (DSTO, nonrecryst.)[42], no ignition[49]
Train test	Ignition (Bofors, nonrecryst.)[42], fails to ignite (DSTO, nonrecryst.)[42], ignited and supported the train steadily[49]

	Fox-7[11]	**Fox-7**[42]	**β-Fox-7**[42]	**γ-Fox-7**[42]
Chemical formula	$C_2H_4N_4O_4$	$C_2H_4N_4O_4$	$C_2H_4N_4O_4$	$C_2H_4N_4O_4$
Molecular weight [g mol^{-1}]	148.09	148.09	148.09	148.09
Crystal system	Monoclinic	Monoclinic	Orthorhombic	Monoclinic
Space group	$P\,2_1/\,n$	$P\,2_1/\,n$	$P\,2_12_12_1$	$P\,2_1/\,n$
a [Å]	6.922(1)	6.941(1)	6.986/(1)	13.354(3)
b [Å]	6.501(1)	6.569(1)	6.660(2)	6.895(1)
c [Å]	11.262(1)	11.315(2)	11.674(3)	12.050(2)
α [°]	90	90	90	90
β [°]	90.485(1)	90.55(2)	90	111.102(8)
γ [°]	90	90	90	90
V [Å^3]	506.77	515.9(1)	543.1(2)	1,035.0(3)
Z	4	4	4	8
ρ_{calc} [g cm^{-3}]	1.941	1.907	1.811	1.901
T [K]	100	173	403	200

Recryst. from dil. hydrochloric acid produces hexagonal-shaped crystals, 100 microns diameter[49]

Summary of exptl. determined unit cell parameters for α-Fox-7[42]:

Sample	Unit cell parameters			
	a (Å)	*b* (Å)	*c* (Å)	*β* (°)
α-Fox-7	6.94	6.56	11.31	90.55
α-Fox-7	6.94	6.64	11.34	90.61
α-Fox-7	6.93	6.62	11.23	89.48
α-Fox-7	6.92	6.55	11.27	90.06

Unit cell parameters of Fox-7 recrystallized under different conditions[36]:

Sample	Unit cell parameters			
	a (Å)	*b* (Å)	*c* (Å)	*β* (°)
Fox-7 recryst. from H_2O	6.946	6.627	11.339	90.54
Fox-7 recryst. from acetone	6.937	6.268	11.317	90.54
Fox-7 recryst. from DMF	6.943	6.627	11.333	90.57
Fox-7 recryst. from DMF/H_2O	6.935	6.623	11.319	90.58
α-Fox-7 (simulated)	6.939	6.651	11.349	90.65

Effect of ultrasound on Fox-7 recrystallization[27]:

Method			Particle size (µm)			Morphology
Application of ultrasound	Scale (g)	Cooling rate (°C/min)	*d*(0.1)	*d*(0.5)	*d*(0.9)	
None	10	0.5	113	278	543	Blocky, jagged
None	100	2.0	86	213	445	Blocky
45 kHz continuous	10	0.5	30	59	105	Rounded, rhombic
45 kHz continuous	10	1.0	–	<60[†]	–	Blocky
45 kHz continuous with surfactant	10	0.5	45	94	183	Rhombic
45 kHz pulsed @ 15 min intervals	100	0.5	48	98	186	Smooth, rhombic
20 kHz continuous	100	0.5	65	105	170	Blocky
20 kHz continuous	100	2.0	27	59	121	Blocky

[†]est. value, agglomeration of particles

Crystallization from H_2O, acetone, DMF is possible and produces α-Fox-7[36], cooling crystallization produces crystals with solvent inclusions with a lower ρ and thermal stability[36]. Heating a crystal with solvent inclusions @ 160 °C shows loss of solvent and β- → γ-phase transition[36]. Product of partial decomposition of Fox-7 recryst. from H_2O shows similar XRD pattern as that of γ-Fox-7[36]

Single crystals can be obtained by slow cooling of Fox-7 solns. in formic acid, acetone, ethanol or a H_2O/acetone mixture[38]

Crystals of 100–600 µm diameter obtained from H_2O/*N*-methyl-2-pyrrolidone (75/25) with 0.3 K/min cooling rate, vigorous mechanical stirring[42]

Crystals of particle diameter 2–18 µm on recryst. from NMP into H_2O @ ambient temperature[42]

Effect of solvent on morphology of Fox-7 crystals; 20 kHz ultrasound was used, 3 g Fox-7 produced[42]:

Solvent	Particle size (µm)			Morphology
	d(0.1)	*d*(0.5)	*d*(0.9)	
NMP/H_2O (50:50)	10	29	66	Sharp blocks
GBL	7	16	30	Rounded plates
DMF	3	11	25	Rounded oblongs
DMF/H_2O (75:25)	12	35	78	Sharp blocks
CH_3CN	30	59	103	Rounded blocks

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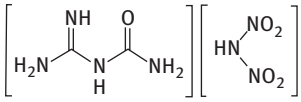
FOX-12

Name [German, acronym]: Guanylurea dinitramide, *N*-guanylurea dinitramide [FOX-12, GUDN]

Main (potential) use: Secondary (high) explosive, air-bag gas generators, promising ingredient for gas generator propellants[10, 11, 20], suitable for melt-cast explosives[11], gun propellants[11], proposed as new ingredient for insensitive high explosive formulations[12], promising oxidizer for propellants, insensitive munitions and airbags[13, 20]

Structural formula:



	FOX-12
Formula	$C_2H_7N_7O_5$
Molecular mass [g mol^{-1}]	209.12
Appearance at RT	Colorless crystals[11], white crystalline[14], white crystalline powder[20], colorless crystalline solid[22]
IS [J]	31 Nm[6], >90[1], drop height >159 cm (BAM apparatus, 2 kg mass)[3, 4], 159 cm[7], 35–50 cm (BAM, depends on morphology)[11], 30 Nm (class 4)[12], 40 Nm (class 1)[12], 50 Nm[13], 35 Nm[13], no reaction under 90 J (BAM)[14], 31 (BAM)[16], 40 Nm[17], >49 (BAM, RT)[18], 49[19, 21], >35 (BAM)[22], 50 (class 4)[22], 35 (propellant grade)[22], 2 m (2 kg mass, BAM)[20], 31[23]
FS [N]	>360[6, 11, 13, 17], >352[1], >350 (Julius-Petri apparatus)[3, 4, 7], <360 (class 4)[12], >360 (class 1)[12], no reaction under 350 N (BAM)[14], >352 (BAM)[16], >353 (Julius Peters, porcelain plate and peg)[18], >353[19, 21], >36 kp (Julius-Peters)[20], >360 (BAM)[23]
ESD [J]	ca. 4.5, >3[1]
N [%]	46.86
$\Omega(CO_2)$ [%]	−19.13
$T_{m.p.}$ [°C]	215[6], 215 (dec.)[16, 23], dec.[19], no mpt. but dec. @ ~180 °C[20]
$T_{phase\ transition}$ [°C]	No phase transitions were found on heating (DSC)[13]

$T_{dec.}$ [°C]	214.8 (onset)[3, 4], ~180[20], 215[7], 214.8 (DSC, onset @ 10 °C/min, E_a = 277 kJ/mol between 200–255 °C)[11], 216.4 (exo, onset), 217.67 (exo, peak max.) (DSC)[13], 206.46 (exo, onset), 210.46 (exo, peak max.) (DSC)[13], 206 (onset, air, DSC @ 10 K/min, propellant grade GUDN)[22], 216 (onset, air, DSC @ 10 K/min, class 4, coarser grade GUDN)[22]		
ρ [g cm^{-3}]	1.75[6, 12, 18, 21], 1.7545 (bulk crystal density from powder X-ray diffraction)[3, 4], 1.75 (X-ray)[8], 1.75 (bulk crystal density @ 20 °C)[10], 1.7545 (crystal, X-ray)[11], 1.7525 (crude, class 2 NSG 120, He pycnometer)[11], 1.742 (@ 298 K)[16], 1.755 (crystal)[22], 1.755 (X-ray)[23], 1.75 (direct)[23]		
Heat of formation	−356 kJ/mol (enthalpy of form.)[6], −355 kJ/mol (bomb calorimetry)[3, 4], −322 kJ/mol (energy of form.)[6], −1,700 kJ/kg (H_f)[10], −356 kJ/mol ($\Delta_f H$)[16, 22], −355 kJ/mol[21], −355.6 kJ/mol (heat of form., $\Delta_f H$)[11, 23], −369.9 kJ/mol ($\Delta_f H$, exptl., bomb calorimeter)[11]		
Heat of combustion	$\Delta H_c°$ = 1,432 kJ/mol[22]		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]	3,512	2,998 [H_2O (L)] (ICT-code)[6] 3,441 [H_2O (g)] (ICT-code)[6] 3.78 k/g (calcd., CHEETAH)[12] 792.2 kJ/mol ($\Delta_{ex}H$)[16], 3.789 kJ g^{-1} ($\Delta_{ex}H$)[16] $\Delta_{ex}H°$ = −811 kJ/mol (@ 1.76 g cm^{-3}) [H_2O (L)][22]	
T_{ex} [K]	2,600	2,887 (@ 1.76 g cm^{-3}, calcd., CHEETAH 2.0)[22] 2,894 (@ 1.75 g cm^{-3})[23]	
$p_{C\text{-}J}$ [kbar]	267	37.5 GPa (calcd., CHEETAH 2.0)[3] 25.5 GPa (@ 1.75 g cm^{-3}, calcd., CHEETAH)[12]	260 261 (@ 1.667 g cm^{-3})[11]

		25.7 GPa (@ TMD, calcd.)[21] 25.89 GPa (@ 1.76 g cm^{-3}, calcd., CHEETAH 2.0)[22] 25.1 GPa (@ 1.75 g cm^{-3})[23]	
VoD [m s^{-1}]	8,380	8,176 (@ 1.666 g cm^{-3}, calcd., BKWR)[9] 8,009 (@ 1.666 g cm^{-3}, calcd., BKWS)[9] 8,210 (@ 1.75 g cm^{-3}, calcd., BKWS)[3, 4] 8,192 (@ 1.75 g cm^{-3}, calcd. CHEETAH)[12] 8,210 (@ TMD, calcd.)[21] 8,235 (@ 1.76 g cm^{-3}, calcd., CHEETAH 2.0)[22] 8,194 (@ 1.75 g cm^{-3})[23]	7,900 7,870 (@ 1.66 g cm^{-3}, 52 × 52 mm uniaxially pressed cylindrical charge)[3, 11] 7,870 (@ 1.66 g cm^{-3})[23]
V_0 [L kg^{-1}]	880		910[2] 785[6]

Exptl. and theoretical detonation performance of beat GUDN compared to the calculated values (CHEETAH 2.0) (* = in copper tube with 6 mm wall thickness)[22]:

Density (g cm^{-3})	Experimental			Calculated	
	V_{CJ} (m/s)	P_{CJ} (GPa)		V_{CJ} (m/s)	P_{CJ} (GPa)
1.670	No det.	No det.	@ 22 mm diameter	7,848	22.57
1.660	7,870	–	@ 52.15 mm diameter	7,806	22.22
1.666	7,966	26.11	@ 60 mm*	7,831	22.43

<table>
<tr><td>Critical diameter [cm]</td><td>Range of 22–54 mm (@ 1.67 g cm^{-3})[22]</td></tr>
<tr><td>Initiation sensitivity</td><td>60 g PETN/FO booster unable to detonate a charge of pressed FOX-12 (Ø = 52.15 mm, ρ = 1.66 g cm^{-3})[11], detonation on increasing booster charge to 300 g[11]

pressed charges: no detonation with 10 g or 50 g boosters[14], detonation observed with 300 g booster[14]</td></tr>
<tr><td>Koenen [mm/type]</td><td>2/F[16]</td></tr>
<tr><td>LSGT [cm]</td><td>sensitivity distance = 18–22.5 mm (72–90 cards) (based on US NOL LSGT, donor charge = RDX pressed with 4% wax, ρ = 1.66 g cm^{-3}, cylinder wall thickness = 3.2 mm, thickness of PMMA disk = 1.5 mm)[11], P_{50} = 6–7 GPa (@ 1.66 g cm^{-3}, NOL-LSGT)[16]

50% probability initiation gap distance = 18–25 mm (59–69 kbar, @ 1.66 g cm^{-3})[22]

50% probability of detonation gap = 18–22.5 mm Gap (FOI-style LSGT)[23]</td></tr>
<tr><td>5 s explosion T [°C]
Explosion T [°C]

Ignition T [°C]</td><td>
192 (Woods metal bath, E_a = 149 kJ/mol between 190–240 °C)[4, 8, 11], 215[23]
No ignition <190 (Wood's metal bath)[11], 200–225[16], 200[19], 216[21]</td></tr>
<tr><td>Thermal stability</td><td>110 °C/400 h[19, 21]</td></tr>
<tr><td>Slow cook-off test (SCO)</td><td>Cook-off @ 144 °C (Fox-12 uniaxially pressed into two cylindrical charges, ~50 mm charge diameter and height, mass of charges = 167 g and 154 g, ρ = 1.66 g cm^{-3}, temperature sensors inside charges, charges enclosed in steel cylinders, heated from 45 °C until reaction @ 3.3 °C/h; type V reaction, that is, burning with no fragmentation of steel cylinder)[11]

IM signature of various GUDN containing stores, Swedish Defence Standard FSD-243, GUDN samples uniaxially pressed into two cylindrical charges, cylinders integrated into steel test vehicles, sample was preheated to 45 °C, then heating @ 3.3 K/h. Samples showed type V reaction, internal T = 144 °C[22]:

<table>
<tr><td>Parameter</td><td>Charge 1</td><td>Charge 2</td></tr>
<tr><td>Height (mm)</td><td>51.52</td><td>47.02</td></tr>
<tr><td>Diameter (mm)</td><td>49.89</td><td>49.87</td></tr>
<tr><td>Weight (g)</td><td>166.92</td><td>153.76</td></tr>
<tr><td>Density (g cm^{-3})</td><td>1.66</td><td>1.67</td></tr>
</table>
</td></tr>
</table>

<table>
<tr><td>Burn rate [mm/s]</td><td>6.0 (@ 7 MPa, Crawford bomb, exptl. burn rate exponent = 0.73)[11], 10.0 mm/s @ 100 atm. pressure[15], 40.0 mm/s @ 500 atm. pressure[15], ~10 mm/s @ 0 MPa[20], ~45 mm/s @ 50 MPa[20], ~75 mm/s @ 100 MPa[19], ~120 mm/s @ 150 MPa[20], 5 mm/s @ 5 MPa[21], 23 m/s @ 50 MPa[21], pressure exponent = 0.7[21]</td></tr>
<tr><td>Flame temperature [K]</td><td>2,680 (calcd.)[11]</td></tr>
<tr><td>Specific impulse (I_{sp}) [s]</td><td>213.1 (calcd.)[11], 196 (formulation with 30% GAP-based binder, calcd.)[11]</td></tr>
<tr><td>Impetus [J/g]</td><td>953 (calcd.)[11]</td></tr>
<tr><td>Particle size [µm]</td><td>Commercially available Fox-12 (EUB): gun propellant grade = 10–25, class 1, NSG 110 = 20–50, class 2, NSG 120 = 80–150, class 4, NSG 140 = 250–400[11], Fox-12 after jet-milling process = 15–20[11]</td></tr>
<tr><td>Solubility [g/mL]</td><td>3.4 g/L in H_2O @ 20 °C[11], more or less insoluble in H_2O[13], 5 g/L in H_2O @ 20 °C[19], very low solubility in cold water[20], moderate solubility in hot water[20], only slightly soluble in water, 3.4 g/L @ 20 °C[22], solubility in DMF = 170 g/L @ 20 °C[22]

Solubility of Fox-12 (g Fox-12/g solvent) @ different temperatures[17]:

<table>
<tr><td rowspan="2">T (°C)</td><td colspan="5">Solvent</td></tr>
<tr><td>DMF</td><td>H_2O</td><td>Acetone</td><td>Ethanol</td><td>Isopropanol</td></tr>
<tr><td>0</td><td></td><td></td><td>0.0</td><td></td><td></td></tr>
<tr><td>10</td><td></td><td></td><td>0.0</td><td></td><td></td></tr>
<tr><td>20</td><td>0.18</td><td>0.0</td><td>0.0</td><td></td><td>0.0</td></tr>
<tr><td>30</td><td>0.22</td><td>0.01</td><td>0.0</td><td></td><td>0.0</td></tr>
<tr><td>40</td><td>0.25</td><td>0.02</td><td>0.0</td><td></td><td>0.0</td></tr>
<tr><td>50</td><td>0.28</td><td>0.03</td><td>0.0</td><td>0.0</td><td>0.0</td></tr>
<tr><td>60</td><td>0.30</td><td>0.04</td><td>0.0</td><td>0.0</td><td>0.0</td></tr>
<tr><td>70</td><td>0.32</td><td>0.07</td><td>0.0</td><td>0.0</td><td>0.0</td></tr>
</table>

solubility (g GUDN/g solvent) in DMF and H_2O @ different T[22]:

<table>
<tr><td>T (°C)</td><td>DMF</td><td>H_2O</td><td>T (°C)</td><td>DMF</td><td>H_2O</td></tr>
<tr><td>20</td><td>0.17 < 0.01</td><td>50</td><td>0.28</td><td>0.02</td><td></td></tr>
<tr><td>30</td><td>0.21</td><td>0.01</td><td>60</td><td>0.29</td><td>0.03</td></tr>
<tr><td>40</td><td>0.25</td><td>0.01</td><td>70</td><td>0.31</td><td>0.05</td></tr>
</table>
</td></tr>
<tr><td>Hygroscopicity</td><td>Nonhygroscopic[13, 20], 0.020% @ 20 °C with 25–75% RH[19]</td></tr>
</table>

<table>
<tr><td>Compatibility</td><td>TAM microcalorimeter @ 75 °C, 19 days, 1:1 weight ratio (substance:Fox12), heat flow limit must remain <63.1 µW/g during 19 days to be considered compatible[11]:
<table>
<tr><th>Fillers</th><th>Binders</th><th>Plasticizers</th></tr>
<tr><td>ADN</td><td>HTPB</td><td>TEGDA</td></tr>
<tr><td>RDX</td><td>3 M GAP</td><td>GAPA</td></tr>
<tr><td>HMX</td><td>GAP 76S04</td><td></td></tr>
<tr><td>Fox-7</td><td></td><td></td></tr>
<tr><td>AP</td><td></td><td></td></tr>
<tr><td>Cl-20</td><td></td><td></td></tr>
</table></td></tr>
<tr><td>pK_a/pK_b</td><td>pK_a (guanylurea) = 11–12[11]</td></tr>
<tr><td>ARC [°C]</td><td>164 (onset), $\phi = 8.3$[16], 163 (onset)[22], 165 (onset for adiabatic self-heating), 179 (deflagration T)[22]</td></tr>
<tr><td>Propellant performance</td><td>Vielle’s law for neat GUDN[22]:
<table>
<tr><th>Pressure range</th><th>A</th><th>n</th><th>Particle size</th></tr>
<tr><td>4–40 MPa</td><td>0.106</td><td>0.989</td><td>–</td></tr>
<tr><td></td><td>1.460</td><td>0.73</td><td>20 µm (propellant grade)</td></tr>
</table></td></tr>
<tr><td>Combustion performance</td><td>Theoretical combustion performance of neat GUDN as calculated with NASA CEA code[22]:
<table>
<tr><th>Unit</th><th>MPa</th><th>0.1</th><th>1</th><th>10</th><th>100</th></tr>
<tr><td>Temperature</td><td>K</td><td>2,126</td><td>2,132</td><td>2,134</td><td>2,135</td></tr>
<tr><td>γ</td><td></td><td>1.2310</td><td>1.2386</td><td>1.2412</td><td>1.2417</td></tr>
<tr><td>MW</td><td>gmol^{-1}</td><td>23.216</td><td>23.229</td><td>23.235</td><td>23.248</td></tr>
<tr><td>CO</td><td>Mol%</td><td>15.499</td><td>15.524</td><td>15.532</td><td>15.518</td></tr>
<tr><td>CO_2</td><td>Mol%</td><td>6.704</td><td>6.692</td><td>6.689</td><td>6.706</td></tr>
<tr><td>H_2</td><td>Mol%</td><td>12.214</td><td>12.231</td><td>12.233</td><td>12.184</td></tr>
<tr><td>H_2O</td><td>Mol%</td><td>26.559</td><td>26.619</td><td>26.639</td><td>26.648</td></tr>
<tr><td>N_2</td><td>Mol%</td><td>38.855</td><td>38.878</td><td>38.885</td><td>38.885</td></tr>
</table></td></tr>
<tr><td>Laser ignition</td><td>No ignition with 100 ms laser pulse ($\lambda = 801$ nm, $M_\lambda = 3.9$ kW cm^{-2}) of consolidated neat class 2 GUDN[22]</td></tr>
</table>

Commercially available crystal grades of GUDN from EURENCO, data from ref.[22]:

Type	Specific surface area ($m^2\ g^{-1}$)	Particle size range (µm)
Propellant grade	0.4–0.6	10–25
Class 1	0.1	25–50
Class 2		80–150
Class 3		Tbd.
Class 4	0.1	250–400

	Fox-12[5]	**Fox-12**[13]	**Fox-12**[13]
Chemical formula	$C_2H_7N_7O_5$	$C_2H_7N_7O_5$	$C_2H_7N_7O_5$
Molecular weight [g mol^{-1}]	209.12	209.12	209.12
Crystal system	Orthorhombic		
Space group	*P n a* 2_1 (no. 33)		
a [Å]	13.660(10)	13.582	13.591
b [Å]	9.3320(10)	9.317	9.308
c [Å]	6.1360(10)	6.238	6.243
α [°]	90		
β [°]	90		
γ [°]	90		
V [$Å^3$]	782.53(16)	789.35	789.82
Z	4		
ρ_{calc} [g cm^{-3}]	1.775	1.76	1.76
T [K]	173		

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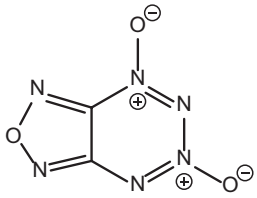
Furazano-1,2,3,4-tetrazine-1,3-dioxide

Name [German, acronym]: [1,2,5]Oxadiazolo[3,4-*e*][1,2,3,4]-tetrazine-4,6-di-*N*-oxide, furazano[3,4-*e*]tetrazine-4,6-dioxide, 5,6-(3,4-furazano)-1,2,3,4-tetrazine-1,3-dioxide [FTDO]

Main (potential) use: Promising candidate for increasing the momentum of propellants and as a component of energetic plasticizers[3, 6]

Structural formula:



	FTDO
Formula	$C_2N_6O_3$
Molecular mass [g mol^{-1}]	156.06
Appearance at RT	Bright yellow crystals[1] orange-yellow needle-like crystals[5], yellow – orange needle-like crystals from recryst. from EtOH/H_2O (2:3), 20–80 µm diameter and 1,000–10,000 µm length[13]
IS [J]	Extremely sensitive[6], impact on pressed charge (charge height = 0.17 mm, rel. ρ = 95%), K-44-PI test machine (load weight = 10 kg, 25 cm drop height) results in detonation in impact region, partial destruction and deformation of rollers, fractured winding of strain gauge[6], H_0 = 30–70 mm (instrument no. 2, lower limit @ P = 2 kg)[13]
FS [N]	120 MPa (under impact shear loading, K-44-II instrument, lower limit)[13]
N [%]	53.85
$\Omega(CO_2)$ [%]	–10.25
$T_{m.p.}$ [°C]	110–112 (dec., crystals; 95–103 crude product)[1, 11], 114 (commercial, crystals, ≥99.0%)[5], 112–113[5], 112.8 (endo peak max., DSC @ 10 °C/min, N_2 atm., 1.12 mg sample)[9], 111.5 (DSC @ 2 °C/min, 1–1.2 mg sample, N_2 atmosphere)[9], 112.0 (DSC @ 4 °C/min, 1–1.2 mg sample, N_2 atmosphere)[9], 112.0 (DSC @ 8 °C/min, 1–1.2 mg sample, N_2 atmosphere)[9], 112.0 (DSC @ 16 °C/min, 1–1.2 mg sample, N_2 atmosphere)[9], 113.0 (DSC @ 32 °C/min, 1–1.2 mg sample, N_2 atmosphere)[9], 112–113.5 (DTA @ 5 K/min)[11], 111–113[12], 112–114 (crystals from EtOH/H_2O (2:3))[13], 113.4 (DSC @ 1 °C/min)[13]
$T_{b.p.}$ [°C]	426 K[2], 200 (@ atmospheric pressure)[9]

$T_{phase\ transition}$ [°C]	Polymorphic transformations not observed during heating up to melting[13]		
$T_{dec.}$ [°C]	140–190 (172.8 °C exo peak max., DSC @ 10 °C/min, N_2 atm., 1.12 mg sample)[9], 153 (exo peak max., DSC @ 2 °C/min, 1–1.2 mg sample, N_2 atmosphere)[9], 159 (exo peak max., DSC @ 4 °C/min, 1–1.2 mg sample, N_2 atmosphere)[9], 172 (exo peak max., DSC @ 8 °C/min, 1–1.2 mg sample, N_2 atmosphere)[9], 179 (exo peak max, DSC @ 16 °C/min, 1–1.2 mg sample, N_2 atmosphere)[9], 190 (exo peak max., DSC @ 32 °C/min, 1–1.2 mg sample, N_2 atmosphere)[9], 146 (DTA @ 5 K/min)[11], 155.8 (DSC @ 1 °C/min)[13], 135 (onset of extensive dec.)[13]		
ρ [g cm^{-3}]	1.85 (not measured)[2], 1.832 ± 0.0011 (@ 20 °C, He pycnometer)[5], 1.828 ± 0.0010 (@ 20 °C, He pycnometer)[5], 1.85[6], 1.84[8], 1.84 (exptl.)[13], 1.852[15]		
Heat of formation	714.3 kJ/mol (ΔH_f (298, liq.), calcd., G3MP2 method)[2], 700.9 kJ/mol (ΔH_f (298, liq.), calcd., G3 method)[2], 691.2 kJ/mol (ΔH_f (298, liq.), calcd., G4MP2 method)[2], 678.3 kJ/mol (ΔH_f (298, liq.), calcd., G4 method)[2], 178.2 kcal/mol (enthalpy of form., calcd., ccCA-P)[3], 174.7 kcal/mol ($\Delta H_f°$(298 K) (g), calcd., ccCA-S3)[3, 11], 176.5 kcal/mol ($\Delta H_f°$(298 K) (g), calcd., ccCA-PS3)[3], 178.3 kcal/mol ($\Delta H_f°$(298 K) (g), calcd., G3)[3, 11], 4,200 kJ/kg (enthalpy of form.)[4], 1,010 ± 26 kcal/kg (enthalpy of form., calcd.)[6], 995 kcal/kg (enthalpy of form.)[6], 172.6 kcal/mol ($\Delta H_f^{gas}{}_{298}$, average calcd. value)[7], 173.9 kcal/mol ($\Delta H_f^{gas}{}_{298}$, calcd., G2)[7], 178.5 kcal/mol ($\Delta H_f^{gas}{}_{298}$, calcd., G3)[7], 170.5 kcal/mol ($\Delta H_f^{gas}{}_{298}$, calcd., CBS-QB3)[7], 172.2 kcal/mol ($\Delta H_f^{gas}{}_{298}$, calcd., G2)[7], 171.7 kcal/mol ($\Delta H_f^{gas}{}_{298}$, calcd., G3)[7], 185.0 kcal/mol ($\Delta H_f^{gas}{}_{298}$, calcd., B3LYP, atomization reaction)[7], 164.4 kcal/mol ($\Delta H_f^{gas}{}_{298}$, calcd., B3LYP)[7], $\Delta H°_f$ = 158 ± 4 kcal/mol (1,010 ± 26 kcal/kg, calcd. in combination with ΔH_{subl})[7, 11], 160.9 kcal/mol ($\Delta H°_f$)[8, 9, 11], 673.2 kJ/mol ($\Delta H_f°$, exptl.)[13], 178.2 kcal/mol (ΔH_f(g)°, calcd., ccCA-P)[14], 174.7 kcal/mol (ΔH_f(g)°, calcd., ccCA-S3)[14], 176.5 kcal/mol (ΔH_f(g)°, calcd., ccCA-PS3)[14], 178.3 kcal/mol (ΔH_f(g)°, calcd., G3)[14], 4,184 kJ/kg ($\Delta H_f°$)[15], 161.02 kcal/mol ($\Delta H_f°$)[16]		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]		7,530 (Q_{cal}, calcd.)[15]	
T_{ex} [K]			
$p_{C\text{-}J}$ [kbar]		40.35 GPa (@ 1.85 g cm^{-3}, heat of form. = 673.7 kJ/mol, calcd.)[2] 40.3 GPa (@ 1.852 g cm^{-3}, calcd.)[15]	

<table>
<tr><td>VoD [m s^{-1}]</td><td></td><td>9,220 (@ 1.85 g cm^{-3}; heat of form. = 673.7 kJ/mol, calcd.)[2]

9,700 (@ 1.84 g cm^{-3} (single crystal ρ), calcd.)[9]

9,600 (@ 1.852 g cm^{-3}, calcd.)[15]</td><td>9,600 (@ 1.55 g cm^{-3} (ρ of pressing), polyethylene tubes 5 mm diameter, 60 mm length)[13]</td></tr>
<tr><td>V_0 [L kg^{-1}]</td><td></td><td></td><td></td></tr>
<tr><td>I_s [Ns g^{-1}]</td><td colspan="3">2.95 (calcd., ISPBKW code)[16], 2.85 (calcd., empirical)[16]</td></tr>
<tr><td></td><td colspan="3"></td></tr>
<tr><td>Critical initiation pressure</td><td colspan="3">0.37 ± 0.02 GPa (disintegrating shell method)[6, 13]</td></tr>
<tr><td>LSGT [cm]</td><td colspan="3">P_{cr} = 0.3 GPa (critical pressure of detonation initiation, calcd., LSGT) [15]</td></tr>
<tr><td>Thermal stability</td><td colspan="3">Can be stored @ 0 °C for a long time[1], crystals (commercial sample, ≥99.0%) stored for >8 years in hermetically sealed glass cans closed with covers with Teflon gasket in dessicator over silica gel @ 18–27 °C showed essentially unchanged properties except decreased ρ[5]

Effect of storage (under laboratory conditions) on ρ (He pycnometer 20 °C)[5]:

<table>
<tr><th>Storage time (years)</th><th>Weighed portion (g)</th><th>ρ (g cm^{-3})</th></tr>
<tr><td rowspan="2">0</td><td>1.0114</td><td>1.832 ± 0.0011</td></tr>
<tr><td>1.0409</td><td>1.828 ± 0.0010</td></tr>
<tr><td rowspan="2">3</td><td>0.9909</td><td>1.809 ± 0.0020</td></tr>
<tr><td>1.0545</td><td>1.810 ± 0.0010</td></tr>
<tr><td rowspan="2">8</td><td>0.8169</td><td>1.788 ± 0.0013</td></tr>
<tr><td>1.0813</td><td>1.787 ± 0.0010</td></tr>
</table>
Est. extent of dec.: 0.11% dec. during 1,385 days[5], 0.23% in 8 years (@ 22 °C, extrapolation based on kinetic data)[5]

(See additional table below detailing the variation in cell parameters on storage time)</td></tr>
<tr><td>Vapor pressure [Pa]</td><td colspan="3">Vapor pressure above liquid FTDO: ln(p [atm]) = –6,391/T + 13.56[9]</td></tr>
<tr><td>Volatility</td><td colspan="3">Able to sublime readily @ RT[13], noticeable weight loss occurs @ 60 °C when the saturation vapor pressure >10 Torr[13]</td></tr>
<tr><td>Burn rate [mm/s]</td><td colspan="3">Combustion @ all pressures accompanied by bright flame[9], in pressure range 0.1–10 MPa combustion law: $u = 18.9p^{0.7}$ [mm/s][9]</td></tr>
</table>

<table>
<tr><td></td><td>Approx. values from graph[9]:

<table><tr><td>u (mm/s)</td><td>p (MPa)</td><td>u (mm/s)</td><td>p (MPa)</td></tr><tr><td>4</td><td>0.1</td><td>55</td><td>3</td></tr><tr><td>5</td><td>0.2</td><td>54</td><td>4</td></tr><tr><td>10</td><td>0.4</td><td>56</td><td>5</td></tr><tr><td>16</td><td>0.6</td><td>60</td><td>6</td></tr><tr><td>21</td><td>1</td><td>80</td><td>9</td></tr><tr><td>18</td><td>1.2</td><td>82</td><td>10</td></tr><tr><td>45</td><td>2.1</td><td></td><td></td></tr></table></td></tr>
<tr><td>Solubility [g/mL]</td><td>g FTDO/100 g solvent @ 20 °C[11]: 66.7 in EtOAc[11], 80 in acetone[11], 89.0 in CH_3CN[11], <0.6 in CCl_4[11], ~0.1 in hexane[11], 0.2 in octane @ 20 °C[11], ~1 in octane @ 80 °C[11] ~45 in 95.6% EtOH[11], 20.0 in 1,2-dichloroethane[11], 17.0 in CH_2Cl_2[11], solubility in H_2O/EtOH mixtures increases as EtOH content increases[11], readily soluble in MeOH, EtOH, ^{i}PrOH, Me_2CO, CH_2Cl_2, $CHCl_3$, $C_2H_4Cl_2$, ethyl acetate, DMF and blended nitramine–nitro ester and nitramine–nitrotriazole plasticizers[13], moderately soluble in benzene, toluene and H_2O[13], poorly soluble in pentane, hexane, heptane and CCl_4[13]</td></tr>
<tr><td>Compatibility</td><td>Partial dec. after heating @ 60 °C in DMF, tetramethylurea or hexamethylphosphoramide for 6 h (UV spec.)[10], dec. occurs actively @ T < 0 °C in more basic solvents such as tributylamine or N-methylmorpholine and sometimes with a flash @ higher T (UV spec.)[10], no noticeable dec. in alphatic acids after 6 h @ 60 °C[10], no reaction with anhydrous alcohols, DMSO or organochlorine solvents after 3 h @ 60 °C (UV spec.)[10], stability in aq. solns. depends on T: no changes in UV after several hours @ 20 °C, essentially no dec. after 3–4 days (UV spec.)[10], inertness in acidic media[11], FTDO forms FTDO-arene solvate systems with, for example, benzene, toluene, o-xylene, nitrobenzene[11], forms solid solns., eutectics and complexes with 2,4-di-nitro-2,4-diazapentane, N,N-bis(β-nitroxyethyl)-nitramine, nitraminopropionitrile, and 4,5-dinitro-2-ethyl-1,2,3-triazole that crystallize from melts[13]</td></tr>
<tr><td>ΔH_{dec} [J/g]</td><td>494 cal/g (DSC @ 10 °C/min)[9], $Q_{dec.}$ = 335 cal/g (DSC @ 4 °C/min, 1–1.2 mg sample, N_2 atmosphere)[9], $Q_{dec.}$ = 805 cal/g (DSC @ 8 °C/min, 1–1.2 mg sample, N_2 atmosphere)[9], $Q_{dec.}$ = 1,047 cal/g (DSC @ 16 °C/min, 1–1.2 mg sample, N_2 atmosphere)[9], $Q_{dec.}$ = 1,011 cal/g (DSC @ 32 °C/min, 1–1.2 mg sample, N_2 atmosphere)[9], 201.14 kJ/mol (DSC @ 1 °C/min)[13]</td></tr>
<tr><td>Effect of excitation by electron beam</td><td>Explosive dec. @ energy ρ of electron beam $H \geq 0.09$ J/cm^2 (FTDO sample pressed @ 400 MPa up to ρ = 1.44 g cm^{-3})[4], explosion initiation probability depends on sample thickness: @ H = 0.27 J/cm^2, sample with 320 µm thickness show initiation probability P = 1[4], but samples with thickness <280 µm did not explode, P = 0 (FTDO sample pressed @ 400 MPa up to ρ = 1.44 g cm^{-3}) [4]</td></tr>
</table>

ΔH_{subl} [kcal/mol]	15.1 ± 0.8 (Burdon manometer, *T* range 40–80 °C)[7, 9]
$\Delta H_{melting}$ [cal/g]	–15.5 (DSC @ 10 °C/min)[9], 7.41 kJ/mol[13]
ΔH_{evap} [kcal/mol]	12.7 (based on heat of melting from DSC)[9]

Variation of unit cell parameters with time of storage under laboratory conditions (X-ray diffraction powder data), crystals obtained by sublimation prior to storage[5]:

Parameter	Storage time (days)			
	0	14	860	1,385
a (Å)	19.893	19.880	20.009	20.061
c (Å)	9.9359	9.9137	10.0259	10.0486
V (Å^3)	3,405.17	3,393.12	3,475.16	3,502.20
Z	24	24	24	24
ρ (g cm^{-3})	1.826	1.833	1.789	1.776

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[13] A. S. Zharkov, P. I. Kalmykov, Y. N. Burtsev, N. P. Kuznetsova, I. A. Merzhanov, N. V. Chukanov, V. V. Zakharov, G. V. Romanenko, K. A. Sidorov, V. E. Zarko, *Russ. Chem. Bull. Int. Ed.*, **2014**, *63*, 1785–1800.
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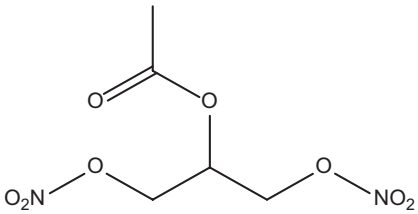
G

Glycerol acetate dinitrate

Name [German, acronym]: Glycerol acetate dinitrate, dinitroacetin, acetyl glycerine dinitrate [acetyldinitroglycerin]

Main (potential) use : Additive to nitroglycerine in order to depress its solidification point[1]

Structural formula:



	Glycerol acetate dinitrate
Formula	$C_5H_8N_2O_8$
Molecular mass [g mol^{-1}]	224.13
Appearance at room temperature (RT)	Colorless and odorless oil (pure)[4]
IS [J]	Very insensitive[4]
N [%]	12.50
$\Omega(CO_2)$ [%]	−42.83
$T_{m.p.}$ [°C]	Not frozen at −20 °C (commercial mixture of isomers)[3], <−20 (freezing point)[5]
$T_{b.p.}$ [°C]	147 (@ 15 mm Hg, commercial mixture of isomers)[3], 147 (@ 15 mm Hg, with dec.)[4], 147 (@ 15 mm Hg)[5]
$T_{dec.}$ [°C]	160 (onset, commercial, mixture of isomers, vigorous dec. @ 170–180 °C)[3], 160 (onset on slow heating in glass tube)[4], 170–180 (vigorous dec. on slow heating in glass tube)[4], 160 (dec. begins) with vigorous dec. @ 179–180 °C[5]
ρ [g cm^{-3}]	1.412[1], 1.462 ± 0.06 (@ 293.15 K)[2], 1.42 (@ 15 °C, commercial, mixture of isomers)[3, 5], sp. gr. = 1.412 (@ 15 °C)[4], sp. gr. = 1.45 (@ 15 °C)[4]
Heat of formation	

https://doi.org/10.1515/9783110672565-007

	Calcd. (K-J)	Lit. values	Exptl.
$-\Delta_{ex}U^{o}$ [kJ kg^{-1}]		2,761.4 J/g (explosion heat)[5] 2,761.4 J/g (explosion heat, commercial, mixture of isomers)[3]	2,761.4 J/g[3] 657 cal/kg [H_2O (gas) @ C^V][4]
T_{ex} [K]			
$p_{C\text{-}J}$ [GPa]			
VoD [m s^{-1}]			
V_0 [L kg^{-1}]			

Trauzl test [cm^3, % TNT]	145 cc (gelatinized: 92% glycerol acetate dinitrate, 8% collodion wool)[4], 200 cm^3 (detonated with no. 8 detonator)[3, 5], 145 cm^3 (blasting gelatin made of 92% acetyl glycerine dintirate)[3, 5]
100 °C heat test [% mass loss]	1.4 % mass loss in 24 h @ 75 °C[4]
Thermal stability	Significant dec. after 24 h @ 75 °C[5, 3]
Volatility	Less volatile than dinitrochlorhydrin[4] but higher than that of dinitroglycerine or NG[4], commercial product is higher than that of NG but lower than that of chloroglycerine dinitrate[5], more volatile than NG (commercial, mixture of isomers)[3]
Solubility [g/mL]	Insoluble in H_2O[4], easily soluble in EtOH, Et_2O, acetone, conc. HNO_3[4], miscible in all amounts with NG[4], miscible with water[5], dissolves NC readily[5]
Compatibility	Gelatinized with collodion wool, can be ignited by impact even at RT [4]
Abel test	Onset after ca. 10 min[4]
Explosion strength	92% that of NG[3]

[1] R. Meyer, J. Köhler, A. Homburg, *Explosives*, 7th edn., Wiley-VCH, Weinheim, **2016**, p. 152.
[2] Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© **1994–2017** ACD/Labs).
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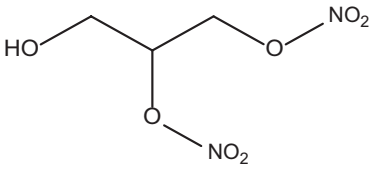
[5] J. Liu, *Nitrate Esters Chemistry and Technology*, Springer, **2019**.

Glycerol 1,2-dinitrate

Name [German, acronym]: Glycerol 1,2-dinitrate*, glyceryl dinitrate, dinitroglycerin, β-isomer of glyceryl dinitrate [glycerin-1,2-dinitrat, 1,2-dinitroglycerin]

Main (potential) use: Gelatinizer of certain types of nitrocelluloses[1], in mixtures for nonfreezing dynamites[5]

Structural formula:



** Glycerol dinitrate often consists of a mixture of the two isomers: 1,2-glycerol dinitrate and 1,3-glycerol dinitrate*[5]

	Glycerol 1,2-dinitrate	
Formula	$C_3H_6N_2O_7$	
Molecular mass [g mol^{-1}]	182.09	
Appearance at RT	Colorless, odorless oil[5]	
IS [J]	1.5 Nm[1], 7–10 cm (2 kg hammer, 1,2- or 1,3-isomer not specified)[7], 30–40 cm (β-isomer, liquid)[7]	
N [%]	15.38	
Ω(CO_2) [%]	–17.6	
$T_{m.p.}$ [°C]	40 (freezing point, 1,2- or 1,3-isomer not specified)[7]	
$T_{dec.}$ [°C]	Distillate hardly decomposed @ 146 °C under 15 mm Hg (1,2- or 1,3-isomer not specified)[7]	
ρ [g cm^{-3}]	1.51[1], 1.594 ± 0.06 (@ 293.15 K)[2], 1.47 (1,2- or 1,3-isomer not specified)[7]	
Heat of formation	–350.6 kJ/mol ($\Delta_f H°$)[3], –1925.4 kJ/kg ($\Delta_f H°$)[3], –472.4 kJ/mol (enthalpy of form., exptl.)[8], –509.6 kJ/mol (enthalpy of form., calcd., emp.)[8]	
	Calcd. (EXPLO5 6.03)	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]	5,702	
T_{ex} [K]	3,803	

$p_{C\text{-}J}$ [GPa]	26.1	
VoD [m s^{-1}]	7,888 (@ TMD)	3,320 (92% glyceryl dinitrate gel, 1,2- or 1,3-isomer not specified)[7]
V_0 [L kg^{-1}]	795	

Trauzl test [cm^3, % TNT]	153% TNT[4], 450 (1,2 or 1,3 isomer not specified)[6], 500 (cf. 82% NG, 1,2- or 1,3-isomer not specified)[7]
5 s explosion *T* [°C] Explosion *T* [°C]	>170 (1,2- or 1,3-isomer not specified)[7]
Solubility [g/mL]	Readily soluble in most organic solvents (1,2- or 1,3-isomer not specified)[7], insoluble in CCl_4 and gasoline (1,2- or 1,3-isomer not specified)[7], solubility in water @ 20 °C = 8.6% (1,2- or 1,3-isomer not specified)[7]
Abel test	Signs of dec. only after 16 days heating (1,2- or 1,3-isomer not specified)[7]

[1] R. Meyer, J. Köhler, A. Homburg, *Explosives*, 7th edn., Wiley-VCH, Weinheim, **2016**, pp. 152–153.
[2] Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© **1994–2017** ACD/Labs).
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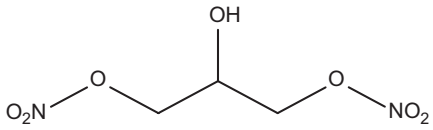
Glycerol 1,3-dinitrate

Name [German, acronym]: Glycerol 1,3-dinitrate*, glyceryl dinitrate, dinitroglycerin, glycerine dinitrate, α-isomer of glyceryl dinitrate [glycerin-1,3-dinitrat, 1,3-dinitroglycerin]

Main (potential) use: Gelatinizer of certain types of nitrocelluloses[1], in mixtures for nonfreezing dynamites[6]

Structural formula:



** Glycerol dinitrate often consists of a mixture of the two isomers: 1,2-glycerol dinitrate and 1,3-glycerol dinitrate*[6]

	Glycerol 1,3-dinitrate	
Formula	$C_3H_6N_2O_7$	
Molecular mass [g mol^{-1}]	182.09	
Appearance at RT	Colorless, odorless oil[6]	
IS [J]	1.5 Nm[1], 90–100 cm for 2 kg weight (α-isomer, hydrate crystals)[5, 8], 30–40 cm for 2 kg weight (β-isomer, liquid)[5], 7–10 cm (2 kg hammer, 1,2- or 1,3-isomer not specified)[8]	
N [%]	15.38	
Ω(CO_2) [%]	−17.6	
$T_{m.p.}$ [°C]	26[2], 40 (freezing point, 1,2- or 1,3-isomer not specified)[8]	
$T_{dec.}$ [°C]	Distillate hardly decomposed @ 146 °C under 15 mm Hg (1,2- or 1,3-isomer not specified)[8]	
ρ [g cm^{-3}]	1.51[1], 1.594 ± 0.06 (@ 293.15 K)[3], 1.47 (@ 20 °C)[5], 1.47 (1,2- or 1,3-isomer not specified)[8]	
Heat of formation	−351.7 kJ/mol ($\Delta_f H°$)[4], −1,931.5 kJ/kg ($\Delta_f H°$)[4]	
	Calcd. (EXPLO5 6.03)	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]	5,695	
T_{ex} [K]	3,800	

$p_{C\text{-}J}$ [GPa]	26.1	
VoD [m s^{-1}]	7,886 (@ TMD)	3,320 (92% glyceryl dinitrate gel, 1,2- or 1,3-isomer not specified)[8]
V_0 [L kg^{-1}]	795	

Trauzl test [cm^3, % TNT]	450 (1,2- or 1,3-isomer not specified)[7], 500 (cf. 82% NG, 1,2 – or 1,3-isomer not specified)[8]
5 s explosion *T* [°C] Explosion *T* [°C]	>170 (1,2- or 1,3-isomer not specified)[8]
Solubility [g/mL]	Readily soluble in most organic solvents (1,2- or 1,3-isomer not specified)[8], insoluble in CCl_4 and gasoline (1,2- or 1,3-isomer not specified)[8], solubility in water @ 20 °C = 8.6% (1,2- or 1,3-isomer not specified)[8]
Abel test	Signs of dec. only after 16 days heating (1,2- or 1,3-isomer not specified)[8]

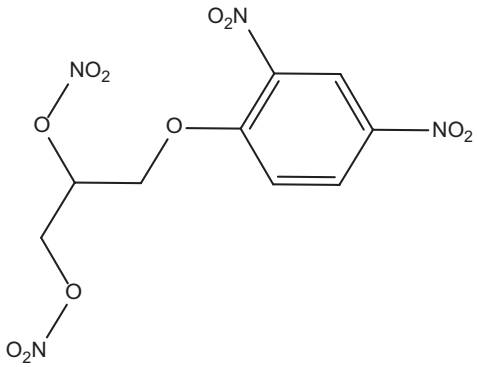
[1] R. Meyer, J. Köhler, A. Homburg, *Explosives*, 7th edn., Wiley-VCH, Weinheim, **2016**, pp. 152–153.
[2] "PhysProp" data were obtained from Syracuse Research Corporation of Syracuse, New York (US).
[3] Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© **1994–2017** ACD/Labs).
[4] G. M. Khrapkovskii, T. F. Shamsutdinov, D. V. Chachkov, A. G. Shamov, *Journal of Molecular Structure (Theochem),* **2004**, *686*, 185–192.
[5] J. Liu, *Liquid Explosives*, Springer-Verlag, Heidelberg, **2015**.
[6] T. L. Davis, *The Chemistry of Powder and Explosives*, *vol. 2*, **1943**, John Wiley and Sons Inc., New York, pp. 214–217.
[7] M. Jafari, M. Kamalvand, M. H. Keshavarz, S. Farrashi, *ZAAC*, **2015**, *641*, 2446–2451.
[8] J. Liu, *Nitrate Esters Chemistry and Technology*, Springer, **2019**.

Glycerol-2,4-dinitrophenyl ether dinitrate

Name [German, acronym]: Glycerol-2,4-dinitrophenyl ether dinitrate [dinitrophenylglycerinetherdinitrat, dinitryl]

Main (potential) use: Gelatinizer of nitrocellulose[1]

Structural formula:



	Dinitryl	
Formula	$C_9H_8N_4O_{11}$	
Molecular mass [g mol^{-1}]	348.18	
Appearance at RT		
IS [J]	8 Nm[1]	
N [%]	16.09	
$\Omega(CO_2)$ [%]	−50.5	
$T_{m.p.}$ [°C]	124[1]	
ρ [g cm^{-3}]	1.667 ± 0.06 (@ 293.15 K)[2]	
Heat of formation		
	Calcd. (K-J)	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]		
T_{ex} [K]		
$p_{C\text{-}J}$ [GPa]		

VoD [m s^{-1}]		
V_0 [L kg^{-1}]		

Trauzl test [cm^3, % TNT]	320 cm^3[3]

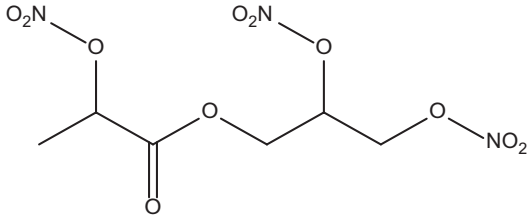
[1] R. Meyer, J. Köhler, A. Homburg, *Explosives*, 7th edn., Wiley-VCH, Weinheim, **2016**, p. 153.
[2] Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© **1994–2017** ACD/Labs).
[3] M. Jafari, M. Kamalvand, M. H. Keshavarz, S. Farrashi, *ZAAC*, **2015**, *641*, 2446–2451.

Glycerol nitrolactate dinitrate

Name [German, acronym]: Glycerol nitrolactate dinitrate, glycerol monolactate trinitrate [dinitroglycerinnitrolactat, GLTN]

Main (potential) use: Gelatinizer of nitrocellulose[1, 5]

Structural formula:



	Glycerol nitrolactate dinitrate	
Formula	$C_6H_9N_3O_{11}$	
Molecular mass [g mol^{-1}]	299.15	
Appearance at RT		
IS [J]	15 cm (1 lb mass, 20 mg sample, B.M.)[5]	
FS [N]	Unaffected by steel shoe (friction pendulum test)[5], unaffected by fiber shoe (friction pendulum test)[5]	
N [%]	14.05	
Ω(CO_2) [%]	−29.4	
ρ [g cm^{-3}]	1.47[1, 3], 1.580 ± 0.06 (@ 293.15 K)[2], 1.47 (liq.)[5]	
Heat of formation		
Heat of combustion	2407 cal/g[5]	
	Calcd. (K-J)	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]		4,837 [H_2O (l)][3] 4,455 [H_2O (g)][3]
T_{ex} [K]		
$p_{C\text{-}J}$ [GPa]		
VoD [m s^{-1}]		
V_0 [L kg^{-1}]		905[3]

Sand test [g]	13.1 g (200 g bomb)[5]
Ballistic mortar test	114% TNT[4]
5 s explosion *T* [°C]	223[5]
100 °C heat test [% mass loss]	2.5% mass loss in first 48 h[5], 1.8% mass loss in second 48 h[5], no explosion in 100 h[5]
Vacuum stability test [cm^3/h]	5.9 cc/40 h @ 100 °C[5]
Volatility [mg/cm^2/h]	28 @ 60 °C[5]
Solubility [g/mL]	<0.01 g/100 g H_2O @ 25 °C[5], >0.015 g in 100 g H_2O @ 60 °C[5]
compatibility	Hydrolysis: 10 days @ 22 °C, 0.021 % acid[5], 5 days @ 60 °C, 0.014% acid[5]
Refractive index	n^D_{25} = 1.464[5]

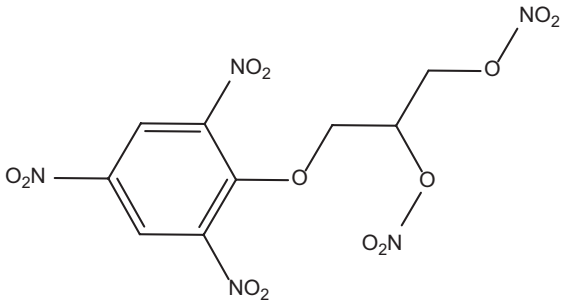
[1] R. Meyer, J. Köhler, A. Homburg, *Explosives*, 7th edn., Wiley-VCH, Weinheim, **2016**, pp. 153–154.
[2] Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© **1994–201**7 ACD/Labs).
[3] J. Köhler, R. Meyer, A. Homburg, *Explosivstoffe*, 10th edn., Wiley-VCH, Weinheim, **2008**, p. 150.
[4] 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**.
[5] *AMC Pamphlet Engineering Design Handbook: Explosive Series Properties of Explosives of Military Interest*, Headquarters, U.S. Army Materiel Command, January **1971**.

Glycerol trinitrophenyl ether dinitrate

Name [German, acronym]: Glycerol trinitrophenyl ether dinitrate
[trinitrophenylglycerinetherdinitrat]

Main (potential) use:

Structural formula:



	Glycerol trinitrophenyl ether dinitrate	
Formula	$C_9H_7N_5O_{13}$	
Molecular mass [g mol^{-1}]	393.18	
Appearance at RT		
IS [J]	4 Nm[1]	
N [%]	17.81	
$\Omega(CO_2)$ [%]	−34.6	
$T_{m.p.}$ [°C]	124[2]	
$T_{dec.}$ [°C]	150[2]	
ρ [g cm^{-3}]	1.782 ± 0.06 (@ 293.15 K)[3]	
Heat of formation		
	Calcd. (K-J)	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]		
T_{ex} [K]		
$p_{C\text{-}J}$ [GPa]		
VoD [m s^{-1}]		
V_0 [L kg^{-1}]		

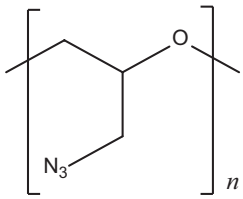
Trauzl test [cm^3, % TNT]	420 cm^3[4]

[1] R. Meyer, J. Köhler, A. Homburg, *Explosives*, 7th edn., Wiley-VCH, Weinheim, **2016**, p. 154.
[2] J. J. Blanksma, P. G. Fohr, *Recueil des TravauxChimiques des Pays-Bas et de la Belgique,* **1946**, *65*, 711–721.
[3] Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© **1994–2017** ACD/Labs).
[4] M. Jafari, M. Kamalvand, M. H. Keshavarz, S. Farrashi, *ZAAC*, **2015**, *641*, 2446–2451.

Glycidyl azide polymer

Name [German, acronym]: Glycidyl azide polymer [glycidylazidpolymer, GAP]
Main (potential) use: Energetic binder for composite propellants[1, 35], energetic polymer[11, 16], active energetic binder in rocket propellants[14], energetic binder/plasticizer in rocket propellant and gas generator applications[15]

Structural formula:



	GAP
Formula	Structural unit: $C_3H_5N_3O$
Molecular mass [g mol^{-1}]	Structural unit: 99.09; mean: 2,000[2], 500–5,000[7], ~700[15], 1,700 ± 300 (GAPdiol)[30], ≥900 (GAPtriol)[30], 508.46 (GAP-A, azido-terminated GAP polymer)[36]
Appearance at RT	Viscous yellow oil (fluid with specific mass of ~1.3 × 10^3 kg/m^3; H-[-O-CH(-CH_2-N_3)-CH_2-]$_n$OH with n = 20, uncured GAP)[13, 14], liquid[33], light yellowish viscous liquid (uncured)[35]
IS [J]	7.9 Nm[1], >170 cm[4], 200 kg/cm[6], 300 kg/cm[7]
FS [N]	>360[1], 32.4 kg[6]
ESD [J]	6.25[2, 6]
N [%]	42.41 (monomer unit)
Ω(CO_2) [%]	−121.1
$T_{m.p.}$ [°C]	177.1 (DSC)[26], 150 (dec.)[35]
$T_{dec.}$ [°C]	253.53 (DSC @ 10 °C min^{-1})[3], 250 (DSC)[6], 255 (TG)[6], 217–218 (ARC combined with DSC)[7], 240 (first stage dec.) and 260–500 (second stage dec.)[7], 215 (RSFTIR @ atmospheric pressure)[7] DTA/TG (He atmosphere, 10.1 MPa, heating rate = 0.167 K/s): 202–227 (exothermic peak, dec. and gasification rxns., corresponds to first stage weight loss of 40% in TG), 227 (second stage weight loss begins without heat liberation)[7], T_i = 187, T_f = 259 (TG, @ 2 °C/min, first stage, GAP prepolymer)[28], T_i = 173, T_f = 254 (TG, @ 2 °C/min, first stage, cross-linked GAP)[28]

DTA/TG (dynamic nitrogen atmosphere, 5 °C/min)[10]:

Heating rate (°C/min)	First stage		Second stage	
	Peak *T* (°C)	Weight loss (%)	Peak *T* (°C)	Weight loss (%)
1	215.4	37.8	314.7	25.1
2	222.9	37.6	323.6	25.2
3	225.6	37.4	325.1	25.1
5	228.9	37.9	334.7	25.3
Average		37.7		25.2

DTA/TG : two-stage dec. process; (i) 475–573 K (exo, 42% mass loss), (ii) *T*> 537 K (exo)[14]

dec. @ 1 bar in Ar, @ 2–5 K/min shows 3 maxima: ~498 K (36 % mass loss), (ii) 608 K, (iii) 698 K (37% more mass loss in stages (ii) and (iii))[14]

184.4 (T_e, onset *T*), 253.7 (T_p, peak max) (DSC @ 10 °C/min, N_2 atmosphere)[19]

Stages of dec.[19]:

Stage 1 dec.			Stage 2 dec.		
DTG	TG		DTG	TG	
T_{p1} (°C)	*T* (°C)	Mass loss (%)	T_{p2} (°C)	*T* (°C)	Mass loss (%)
238.7	277.7	39.3	337.3	850.0*	57.8

* This value may be incorrect.

DSC @ different pressures[19]: 253.7 (exo, peak max, DSC @ 0.1 MPa pressure, 10 °C/min)[19], 252.7 (exo, peak max, DSC @ 2 MPa pressure, 10 °C/min)[19], 249.6 (exo, peak max, DSC @ 6 MPa pressure, 10 °C/min)[19]

Heating rate (°C/min)	Dec. onset *T* (°C)	Dec. *T* (°C)	Dec. final *T* (°C)
1	192	223	240
1.5	195	228	242
2	196	229	245
2.5	200	235	251

TGA[29]: T_m (max reaction *T*), T_o (onset *T*), DSC @ 10 °C/min[29]: $T_o = 233$, $T_m = 251$ (GAP prepolymer, uncured)[29], $T_o = 233$, $T_m = 240$ (GAP binder, cured)[29]

$T_{glass\ transition}$ [°C]	−43[7], −20 – 50 (linear)[7], −49.2 ± 0.4 (DSC, GAP average MW = 1534 g/mol)[12], −48[23, 24], 228 K (DSC @ 20 °C/min)[29], −45 (GAP diol)[30], −45 (GAP triol)[30], −50[32], −78.8 (GAP-A, azido-terminated GAP)[36]		
ρ [g cm^{-3}]	1.29[1, 35], 1.30[2, 7, 11, 31, 32], 1.3 (n = 20, uncured)[14], 1.27 (GAP polymer $C_{3.3}H_{5.6}O_{1.12}N_{2.63}$)[16], 1.27[25], 1.29 (GAP diol)[30], 1.29 (GAP triol)[30], 1.27 (GAP-A, azido-terminated GAP polymer)[36] Values cited in ref.[27]:1.275[27], 1.27[27], 1.23[27], 1.28[27], 1.3[27]		
Heat of formation	114 kJ/mol (enthalpy of form.)[1], 1150 kJ/kg (enthalpy of form.)[1], 176 kJ/mol[31], 67.89 kcal/mol (dimer unit, ΔH_f (g))[9], 340 kcal/mol (ΔH_f (l), 2,200 g/mol polymer, exptl. value)[9], 746.79 kcal/mol (ΔH_f (g), 2,200 g/mol polymer, calcd. value)[9], 169.7 kcal/mol (ΔH_f (g), 500 g/mol polymer, calcd. value)[9], 584.90 kcal/mol (ΔH_f (l), 2200 g/mol polymer, calcd. value)[9], 120.96 kcal/mol (ΔH_f (l), 500 g/mol polymer, calcd. value)[9], 0.23 kcal/kg (ΔH_f)[15], 0.28 kcal/kg (ΔH_f)[15], 0.33 kcal/kg (ΔH_f)[15], 957 kJ/kg (ΔH_f)[16, 27], 957 kJ/kg[11], 0.25 kJ/g (ΔH_f°, GAP 900)[17], 0.34 kJ/g (ΔH_f°, GAP 1300)[17], 1.15 kJ/g (ΔH_f°, GAP 2,900)[17], 1.170 kJ/g (ΔH_f°, GAP prepolymer, *Frankel*)[17], 0.957 kJ/g (ΔH_f°, GAP prepolymer, *Kubota*)[17], 1.394 kJ/g (ΔH_f°, GAP prepolymer, *Rhein*)[17], 1.423 kJ/g (ΔH_f°, GAP prepolymer, *Meyer*)[17], 1.201 kJ/g (ΔH_f°, GAP prepolymer, *Phatak*)[17], 1.434 kJ/g (ΔH_f°, GAP prepolymer, CHEETAH 2.0)[17], 957 kJ/kg[23, 24], 1,150.2 kJ/kg[25], 117 kcal/mol (GAP diol)[30], 117 kcal/mol (GAP triol)[30], 117 kJ/mol[32], 0.957 MJ/kg ($\Delta H_{f,r}$, 293 K, GAP prepolymer)[33], 114 kJ/mol (enthalpy of form.)[35], 141.0 kJ/mol (enthalpy of form., exptl.)[37], 109.8 kJ/mol (enthalpy of form., calcd., emp.)[37] Heat of formation values cited in ref.[27]: 254.7 kJ/kg[27], 322 kJ/kg[27], 611 kJ/kg[27], 1,171 kJ/kg[27], 1,380 kJ/kg[27]		
Heat of combustion	957 kJ/kg (monomer)[8], 474 cal/g[7], 28.4 kcal/mol (linear)[7], 42 kcal/mol (branched)[7], 4.78 kcal/g (500 g/mol polymer, calcd.)[9], 4.8 kcal/g (500 g/mol polymer, exptl.)[9], 5,010 ± 15 cal/g[7], −20.0 kJ/g ($\Delta_c H$°, GAP 900)[17], −20.1 kJ/g ($\Delta_c H$°, GAP 1300)[17], −20.3 kJ/g ($\Delta_c H$°, GAP 2900)[17]		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{ex}U$° [kJ kg^{-1}]	3,824	3,430 [H_2O (l)][35]	3,429 [H_2O (l)][1]
T_{ex} [K]	2,469		
$p_{C\text{-}J}$ [GPa]	12.9		
VoD [m s^{-1}]	6,597 (@ 1.293 g cm^{-3})		
V_0 [L kg^{-1}]	793		946[1, 5]

<table>
<tr><td>Thermal stability</td><td>GAP is stable up to ~343 K, but begins to slowly lose weight above this T[15]

Gas evolution from GAP sample $[OCH_2CH(CH_2N_3)]_nOH$ (average molecular weight of sample = 2,300, synthesized @ 115 °C, time of PECH azidation = 8 h, gas evolution is highly dependent on sample preparation process and average molecular weight)[18]:

<table>
<tr><td>@ 80 °C</td><td>Time (min)</td><td>Gas evolution (ΔV, cm^3/g)</td><td>@ 95 °C</td><td>Time (min)</td><td>Gas evolution (ΔV, cm^3/g)</td></tr>
<tr><td></td><td>0</td><td>0</td><td></td><td>0</td><td>0</td></tr>
<tr><td></td><td>1,000</td><td>~ 0.06</td><td></td><td>~ 300</td><td>~ 0.075</td></tr>
<tr><td></td><td>2,000</td><td>0.1</td><td></td><td>~ 500</td><td>~ 0.13</td></tr>
<tr><td></td><td>5,000</td><td>~ 1.6</td><td></td><td>~ 600</td><td>~ 0.2</td></tr>
<tr><td></td><td>7,000</td><td>~ 1.9</td><td></td><td>~ 1500</td><td>~ 0.28</td></tr>
<tr><td></td><td>~ 8,750</td><td>~ 2.1</td><td></td><td>~ 2,000</td><td>~ 0.31</td></tr>
</table>
</td></tr>
<tr><td>Vacuum stability test [cm^3/h]</td><td>0.4 ± 0.1 mL/g[21]</td></tr>
<tr><td>Burn rate [mm/s]</td><td>2.2 mm/s (@ 4.5 bar) –11 mm/s (@ 80 bar) (initial T, T_0 = 293 K, cured GAP in N_2 atmosphere)[14], 18.3 (uncured GAP in Ar @ 1 bar, quartz vial, 8 mm diameter)[14]

GAP binder[16]:

<table>
<tr><td>Burn rate × 10^3 (m/s)</td><td>Pressure (MPa)</td></tr>
<tr><td>~5.5</td><td>~ 0.65</td></tr>
<tr><td>~6</td><td>~ 0.8</td></tr>
<tr><td>~7</td><td>~ 1</td></tr>
<tr><td>~9</td><td>~ 2</td></tr>
<tr><td>~10</td><td>~ 2.5</td></tr>
</table>

1.35 (@ 1 atm., SMATCH/FTIR spectroscopy)[34], 1.7 (@ 1 atm., strand burner)[34]</td></tr>
<tr><td>Flame T [K]</td><td>1,300[15], 1,365 @ 735 psi[15], 1,465 (@ 5 MPa)[16], 1,365 (@ 5 MPa, GAP polymer, $C_{3.3}H_{5.6}O_{1.12}N_{2.63}$)[16], 1,890 (GAP binder)[16], 1,470 (@ 5 MPa, GAP prepolymer)[33], 1,370 (@ 5 MPa, GAP copolymer)[33]</td></tr>
</table>

<table>
<tr><td>Surface T during combustion [K]</td><td>700–765[15], 710–750[15], 813[15]</td></tr>
<tr><td>Viscosity [cP]</td><td>500–5,000[7], 2.4 × 10^3 @ 25 °C[23]</td></tr>
<tr><td>Hygroscopicity</td><td>Hygroscopic[12]

Moisture content of GAP as function of environmental exposure time[12]:

<table><tr><td>Time (h)</td><td>Moisture (%)</td></tr><tr><td>0</td><td>~0.25</td></tr><tr><td>~0.5</td><td>~0.35</td></tr><tr><td>~1</td><td>~0.45</td></tr><tr><td>~1.5</td><td>0.065</td></tr><tr><td>~24</td><td>~0.13</td></tr><tr><td>192</td><td>>0.5</td></tr></table></td></tr>
<tr><td>Compatibility</td><td>Incompatible with CL-20 (lowers thermal stability of CL-20)[21], CL-20 unstable when mixed with isocyanate-cured GAP[21], CL-20 is compatible with GAP[21], good compatibility with high-energy oxidizers like AP and ADN[24]</td></tr>
<tr><td>ARC (accelerated rate calorimetry)</td><td>m/g = 0.1, T_0 (onset T) = 163 ± 4 °C, −ΔM (mass loss) = 34%, P_r (residual pressure) = 0.4 MPa, E (activation energy) = 110 ± 4 kJ mol^{-1}, ln(Z/min^{-1}) (Z = preexponential factor) = 26 ± 1[22]</td></tr>
<tr><td>Thermal conductivity [cal/cm-s-K]</td><td>3.5 × 10^{-4}[27], 5.76 × 10^{-4}[27]</td></tr>
<tr><td>Heat capacity [cal/g-K]</td><td>0.45[27]</td></tr>
<tr><td>Activation energy for initial dec. stage [kcal/mol]</td><td>Values cited in ref.[27]: 43 (TG)[27], 41.5 (DSC)[27], 41.6 (DTA, TG)[27], 37 (TGA)[27], 39.9 and 41.9 (theoretical)[27], 32.4 (TGA, DSC)[27], 39.4 ± 0.3 (TGA)[27], 43.2 ± 2.8 (SMATCH)[27], 42.2 (MS)[27], 43.5 (DSC)[27], 39.3 (MBMS)[27]</td></tr>
<tr><td>Dec. enthalpy, ΔH [J/g]</td><td>440 (cross-linked GAP, DSC @ 2 °C/min)[28], 550 cal/g (DSC @ 10 °C/min, GAP prepolymer, uncured)[29], 474 cal/g (DSC @ 10 °C/min, GAP binder, cured)[29]</td></tr>
</table>

[1] R. Meyer, J. Köhler, A. Homburg, *Explosives*, 7th edn., Wiley-VCH, Weinheim, **2016**, p. 154.
[2] M. B. Frankel, L. R. Grant, J. E. Flanagan, *Journal of Propulsion and Power*, **1992**, *8*, 560–563.
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[10] S.-F. Lu, *Mechanisms and Kinetics of Thermal Degradation of Glycidyl Azide Polymer*, ICT **2016**, Karlsruhe, Germany, pp. 41-1–41-12.
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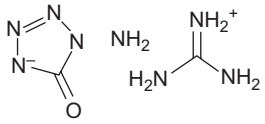
Guanidinium 1-aminotetrazol-5-oneate

Name [German, acronym]: Guanidinium 1-aminotetrazol-5-oneate [ATO-G]
Main (potential) use: Secondary (high) explosive
Structural formula:



	ATO · G		
Formula	$C_2H_8N_8O$		
Molecular mass [g mol^{-1}]	160.16		
Appearance at RT	White powder[1]		
IS [J]	>40[1]		
N [%]	69.97		
$\Omega(CO_2)$ [%]	−74.0		
$T_{m.p.}$ [°C]	184.5 (DSC-TG @ 10 °C/min)[1]		
$T_{dec.}$ [°C]	224.8 (DSC-TG @ 10 °C/min)[1]		
ρ [g cm^{-3}]	1.569 (@ 298 K)[1]		
Heat of formation	286.5 kJ/mol ($\Delta_f H°$)[1], 1790.6 kJ/kg ($\Delta_f H°$)[1]		
	Calcd. (EXPLO5 6.04)	Calcd. (K-J)	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]	3,691		
T_{ex} [K]	2,436		
$p_{C\text{-}J}$ [GPa]	25.4	25.0[1]	
VoD [m s^{-1}]	8,614 (@ 1.569 g cm^{-3}, $\Delta_f H$ = 286.5 kJ mol^{-1})	7,830[1]	
V_0 [L kg^{-1}]	938		

	ATO-G[1]
Chemical formula	$C_2H_8N_8O$
Molecular weight [g mol^{-1}]	160.16
Crystal system	Monoclinic
Space group	*C*2/*c*
a [Å]	12.7785(11)
b [Å]	6.4100(6)
c [Å]	16.5787(15)
α [°]	90
β [°]	93.3030(10)
γ [°]	90
V [Å^3]	1,355.7(2)
Z	8
ρ_{calc} [g cm^{-3}]	1.569
T [K]	298

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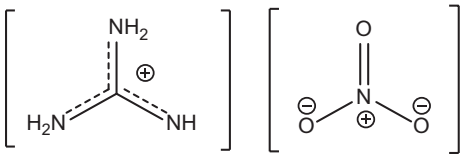
Guanidinium nitrate

Name [German, acronym]: Guanidine nitrate [guanidinnitrat, GuN]
Main (potential) use: Precursor in the synthesis of nitroguanidine[1, 11], ingredient of some blasting explosives, component of fusible explosive mixtures containing AN[10], important intermediate product in the commercial manufacture of NQ and aminoguanidine[10], main use is in propellant compositions[15], has been used as component of high explosive mixtures[15] smoke and gas generating pyrotechnic compositions[18], starting material for production of NQ[18]

Structural formula:



	Guanidine nitrate
Formula	$CH_6N_4O_3$
Molecular mass [g mol^{-1}]	122.08
Appearance at RT	Crystalline[10, 11], white crystalline material[15], white granules[16], colorless crystals/white powder[18]
IS [J]	>5 Nm[1], no detonation on 10 kg mass falling 3.1 m[8], ≥135 kJ/m^2 (pure sample)[19], 71 kJ/m^2 (technical grade)[19]
FS [N]	>353[1], 844 MPa @ 2.4 m/s (pure sample)[19], ≥729 MPa @ 2.4 m/s (technical grade)[19], ≥847 MPa @ 3.0 m/s (technical grade)[19]
ESD [J]	1.26 (pure sample)[19], 0.075 (technical grade)[19]
N [%]	45.89
$\Omega(CO_2)$ [%]	−26.2
$T_{phase\ transition}$ [°C]	296 K (GuN-I → GuN-II)[20], 348 K (GuN-II → GuN-III)[20]
$T_{m.p.}$ [°C]	213[2, 9], 215[1], 468 K[7], 214.2 (crystals)[8], 215–216[10, 11], 213 (endo, onset), 217 (endo, peak max.) (DSC @ 20 °C/min)[14], 206–216[15], 206–212[16], 220[18]

$T_{dec.}$ [°C]	302 (DSC @ 5 °C/min)[2], 354 (exo, onset), 401 (exo, peak max.) (DSC @ 20 °C/min)[14]		
ρ [g cm^{-3}]	1.436[1], 1.44[3, 18], sp. gr. = 1.436 (@ 30°)[8]		
Heat of formation	−407.2 kJ/mol (enthalpy of form., calcd., emp.)[4], −387.1 kJ/mol (enthalpy of form., exptl.)[4], −348.6 kJ/mol (enthalpy of form., calcd., S-D method)[4], −3,170.1 kJ/kg (enthalpy of form.)[1], 712.8 kcal/kg[17], 88–97 kcal/mol[8], −92.48 kcal/mol ($\Delta H°_f$, exptl.)[12], −91.94 kcal/mol ($\Delta H°_f$, calcd.)[12], −92.48 kcal/mol ± 0.13($\Delta H°_f$)[13], −387 kJ/mol (enthalpy of form.)[18]		
Heat of combustion	1,715 cal/g (@ C^V, H_2O (l))[8], 1,716 kcal/kg (@ C^V)[17]		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]	5,216	1,870 [H_2O (g)][18]	2,455 [H_2O (l)][1] 1,871 [H_2O (g)][1]
T_{ex} [K]	3,370		
$p_{C\text{-}J}$ [GPa]	23.1		
VoD [m s^{-1}]	7,075 (@ 1.43 g cm^{-3}; $\Delta_f H = -390$ kJ mol^{-1})		3,700[8] Not determined since only partial detonation could be achieved[10] 3,700 (@ 1.9 g cm^{-3}, brought to detonation in steel tube (36/42 mm) by using 50 g NP/Mn (95/5))[10]
V_0 [L kg^{-1}]	1,002		1,083[1]

Trauzl test [cm^3, % TNT]	10% TNT[8], 140 cm^3[10], 110 cm^3 (*Kast*)[10]
Initiation efficiency	Can only be detonated with difficulty[10]
Vapor pressure [atm. @ °C]	2.66×10^{-18} Pa @ 25 °C[9]
Solubility [g/mL]	Readily soluble in EtOH[11], very readily soluble in H_2O[11, 18], soluble in H_2O (4.64 g in 100 mL H_2O)[10], soluble in EtOH[10], readily soluble in H_2O[15], moderately soluble in EtOH[15]

Hygroscopicity	not deliquescent[11], nonhygroscopic[16]
Heat of melting [J/g]	186 (DSC @ 20 °C/min)[14]
Heat of dec. [J/g]	1,979 (DSC @ 20 °C/min)[14]
Dust explosion	≥4.1 kg/m^3 (technical grade)[19]

Transition and propagation data from ref.[19]:

Sample	Initiation source	Simulated mix	Test sensing	Temperature	Container size (in)	Critical ht. or critical diam. (in)	Velocity	Remarks
					Transition	C_H		
Technical-grade GN	12 g bag igniter	Dryer	Visual	Ambient	1 × 24 (2.54 cm × 61 cm)	≥24 (61 cm)	–	Smoke, muffle noise, sample scattered
Technical-grade GN	12 g bag igniter	Dryer	Visual	Ambient	2 × 24 (5.1 × 61 cm)	≥24 (61 cm)	–	Smoke, muffle noise, sample scattered

Detonation velocity of technical grade guanidine nitrate – witness plate data, data from ref.[19]:

Alum (62 mls)	Approx. diam. of depression inches	Guanidine nitrate (GMS)	Approx. depth of depression inches	Time over 1 ft in ms (1×10^{-6})	Rate (m/s)	Results
No	1.125 (2.86 cm)	140	0.195 (0.50 cm)	111.2	2.741	Hi order Lg frag
No	1.125 (2.86 cm)	146	0.175 (0.44 cm)	109.2	2.791	Hi order Lg frag
No	1.063 (2.70 cm)	148	0.165 (0.42 cm)	108.6	2.807	Hi order Lg frag

Yes	1.000 (2.54 cm)	145	0.130 (0.33 cm)	109.7	2.778	Hi order Lg frag
Yes	0.750 (1.91 cm)	146	0.100 (0.25 cm)	111.6	2.731	Hi order Lg frag
Yes	1.000 (2.54 cm)	142	0.120 (0.30 cm)	112.0	2.721	Hi order Lg frag

2.762 m/s average

Propagation characteristics of guanidine nitrate/water mixtures, data from ref.[19]:

Mixture composition (wt.%)		Propagation test results pipe, diameter (in)			
GN	H_2O	1.0	1½	2	2½
100	0	y	y	y	y
95	5	n*			
85	15	n	y*		
80	20			y	
75	25			y	
70	30			n	
60	40			n	

n* = did not propagate or incomplete propagation; y = detonated completely

	GuN[5]	GuN[6]	GuN[6]	GuN[6]	GuN[6]	GuN[6]	GuN[7]	GuN[7]	GuN[7]	GuN[7]
							Diamond anvil cell, 0.36 GPa pressure	Diamond anvil cell, 0.68 GPa pressure		1.51 GPa pressure
Chemical formula	$CH_6N_4O_3$	$CH_6N_4O_3$	$CH_6N_4O_3$	$CH_6N_4O_3$	$CH_6N_4O_3$	$CH_6N_4O_3$	$CH_6N_4O_3$	$CH_6N_4O_3$	$CH_6N_4O_3$	$CH_6N_4O_3$
Molecular weight [g mol^{-1}]	122.10	122.10	122.10	122.10	122.10	122.10	122.10	122.10	122.10	122.10
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	*C m* (no. 8)	*C m* (no. 8)	*C* 2/ *m* (no. 12)	*C m* (no. 8)	*C m* (no. 8)	*C m* (no. 8)	*C* 2/*m*	*P c* (no. 7)	*C m* (no. 8)	*P c* (no. 7)
a [Å]	12.686(3)	12.545(5)	12.616(33)	12.714(5)	12.706(7)	12.710(6)	12.340(3)	4.8990(10)	12.686(8)	4.8670(10)
b [Å]	7.274(2)	7.303(4)	7.283(5)	7.273(3)	7.260(4)	7.268(4)	7.2110(14)	4.9170(10)	7.272(4)	4.8450(10)
c [Å]	3.629(1)	7.476(4)	7.592(20)	3.5356(9)	3.6077(9)	3.5561(4)	7.3900(15)	10.350(2)	3.6291(18)	10.140(2)
α [°]	90	90	90	90	90	90	90	90	90	90
β [°]	120.85(2)	124.93(5)	123.88(29)	121.28(3)	121.01(4)	121.18(4)	125.00(3)	100.80(3)	120.85(6)	102.91(3)
γ [°]	90	90	90	90	90	90	90	90	90	90
V [Å^3]	287.5	561.535	579.128	279.41	285.23	281.046	538.67(19)	244.90(9)	287.425	233.06(8)
Z	2	4	4	2	2	2	4	2	2	2
ρ_{calc} [g cm^{-3}]		1.444	1.4	1.451	1.421	1.443	1.506	1.656	1.411	1.740
T [K]		295	391	153	257	185	295	295	295	295

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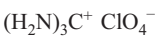
Guanidinium perchlorate

Name [German, acronym]: Guanidine perchlorate [guanidinperchlorat]
Main (potential) use: Suggested as an ingredient of explosive mixtures
Structural formula:



	Guanidinium perchlorate	
Formula	$CH_6N_3O_4Cl$	
Molecular mass [g mol^{-1}]	159.53	
Appearance at RT	Colorless crystals[16]	
IS [J]	50 cm (2 kg mass, B.M.)[5], $H_{50\%}$ = >5 cm (2 kg mass, B.M.)[14], 605 explosions for 2 kg mass falling 250 mm[15], 50% explosions for 124 kg cm[15]	
N [%]	26.34	
$\Omega(CO_2)$ [%]	−10.0	
$T_{phase\ transition}$ [°C]	180–182 (endotherm, DTA, observed as exotherm in DTA cooling curve)[15], cubic crystals above and below transition *T*[15], 180 (DTA, Ar atmosphere, cubic → cubic)[16]	
$T_{m.p.}$ [°C]	248 ± 2[1, 5], 240[4, 15, 16], 526 K[8], 250[11], 248 ± 2 (endo, DTA)[15], 237[15], 255 (DTA, Ar atmosphere)[16]	
$T_{dec.}$ [°C]	337[2] (explodes ~367)[5], 300 (slow dec., DTA)[15], 392 (exotherm, DTA)[15], 275–325 (TG, Ar atmosphere)[16], 310 (DTA, Ar atmosphere)[16]	
ρ [g cm^{-3}]	1.1398 (@ 298.15 K)[3], 1.82[4], sp. gr. = 1.1–1.67[5], 1.772 (calcd., X-ray)[15], 1.743 (measured)[15]	
Heat of formation	−311.1 kJ/mol (enthalpy of form.)[4], −1950.0 kJ/kg (enthalpy of form.)[4], −74.10 ± 0.55 kcal/mol[15], −74.25 kcal/mol ($\Delta H°_f$, exptl.)[13], −75.25 kcal/mol ($\Delta H°_f$, calcd.)[13], −74.10 ± 0.55 kcal/mol (ΔH_f)[15]	
	Calcd. (EXPLO5 6.03)	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]	4,091	
T_{ex} [K]	3,499	
$p_{C\text{-}J}$ [GPa]	9.5	

VoD [m s^{-1}]	5,632 (@ TMD)	7,150 (@ 1.67 g cm^{-3})[10] 6,000 (@ 1.15 g cm^{-3})[11, 12] 6,000 (@ sp. gr. = 1.15)[5] 7,150 (@ sp. gr. = 1.67)[5]
V_0 [L kg^{-1}]	914	

Trauzl test [cm^3, % TNT]	130% TNT[10], 440 cc (10 g sample)[5], 400 cm^3[11, 12]
Ballistic mortar test	124% TNT[10]
Shock sensitivity	Moderately sensitive[11], similar sensitivity cf. PA[11]
5 s explosion *T* [°C] Explosion *T* [°C] Ignition *T* [°C]	 Explosive dec. if heated >300 °C[11] 367[15]
Thermal stability	Slight mass loss occurs on heating @ $T \leq 300$ °C for several hours @ 1 atm. pressure[15], complete dec. @ *T* between 300 and 400 °C[15], air stable crystals[16]
Flame *T*	Calcd. flame *T* as monopropellant and as a component of stoichiometric mixtures with a high-grade paraffin as fuel ($(CH_2)_n$ with $\Delta H_f = -5.971$ kcal/mol @ 298 K)[15]:

Monopropellant combustion		Stoichiometric combustion	
T (K), 1 atm	*T* (K), 1,000 psi	*T* (K), 1,000 psi	S. I., lb s lb^{-1}
2,253	2,325	3,126	263.6

Solubility [g/mL]	31% by wt. in water @ 25 °C[15], 40.3% by wt. in acetone @ 25 °C[15], insoluble in nonpolar solvents[15]
Hygroscopicity	Nonhygroscopic[11, 15, 16]
Compatibility	Not hydrolyzed in aqueous soln.[15], thermal dec. catalyzed by metal oxides[15]

	Guanidinium perchlorate [6, 7]	Guanidinium perchlorate[8]	Guanidinium perchlorate[8]	Guanidinium perchlorate[8]	Guanidinium perchlorate[8]	Guanidinium perchlorate[8]	Guanidinium perchlorate[8]	Guanidinium perchlorate[8]	Guanidinium perchlorate[8]	Guanidinium perchlorate[8]
Chemical formula	$CH_6N_3O_4Cl$	$CH_6N_3O_4Cl$	$CH_6N_3O_4Cl$	$CH_6N_3O_4Cl$	$CH_6N_3O_4Cl$	$CH_6N_3O_4Cl$	$CH_6N_3O_4Cl$	$CH_6N_3O_4Cl$	$CH_6N_3O_4Cl$	$CH_6N_3O_4Cl$
Molecular weight [g mol^{-1}]	159.54	159.54	159.54	159.54	159.54	159.54	159.54	159.54	159.54	159.54
Crystal system	Rhombohedral	Hexagonal	Hexagonal	Hexagonal	Hexagonal	Hexagonal	Hexagonal	Hexagonal	Hexagonal	Hexagonal
Space group	*R* 3 (no. 146)	*R* 3 *m* (no. 160)	*R* 3 *m* (no. 160)	*R* 3 *m* (no. 160)	*R* 3 *m* (no. 160)	*R* 3 *m* (no. 160)	*R* 3 *m* (no. 160)	*R* 3 *m* (no. 160)	*R* 3 *m* (no. 160)	*R* 3 *m* (no. 160)
a [Å]	7.606(2)	7.5826(3)	7.56586(15)	7.5940(6)	7.57142(15)	7.5566(2)	7.5590(2)	7.5643(3)	7.58491(19)	7.6045(3)
b [Å]	7.606(2)	7.5826(3)	7.56586(15)	7.5928(5)	7.57142(15)	7.5566(2)	7.5590(2)	7.5643(3)	7.58491(19)	7.6045(3)
c [Å]	9.121(2)	9.0356(4)	8.8972(3)	9.1179(7)	8.9748(2)	8.8263(3)	8.8537(3)	8.9165(4)	9.0692(3)	9.1725(59)
α [°]	90	90	90	90	90	90	90	90	90	90
β [°]	90	90	90	90	90	90	90	90	90	90
γ [°]	120	120	120	120	120	120	120	120	120	120
V [Å^3]	456.968	449.91(3)	441.065(18)	455.30(6)	445.565(17)	436.47(2)	438.11(2)	441.84(3)	451.86(2)	459.37(4)
Z	3	3	3	3	3	3	3	3	3	3
ρ_{calc} [g cm^{-3}]	1.739	1.766	1.802	1.746	1.784	1.821	1.814	1.799	1.759	1.730
T [K]	295	250	150	300	210	100	125	175	270	325

	Guanidinium perchlorate[8]	Guanidinium perchlorate[8]	Guanidinium perchlorate[9]	Guanidinium perchlorate[9]	Guanidinium perchlorate[9]	Guanidinium perchlorate[9]	Guanidinium perchlorate[9]
			Diamond anvil cell, 0.38 GPa pressure	Diamond anvil cell, 0.57 GPa pressure	Diamond anvil cell, 1.03 GPa pressure	Diamond anvil cell, 1.35 GPa pressure	Diamond anvil cell, 1.73 GPa pressure
Chemical formula	$CH_6N_3O_4Cl$	$CH_6N_3O_4Cl$	$CH_6N_3O_4Cl$	$CH_6N_3O_4Cl$	$CH_6N_3O_4Cl$	$CH_6N_3O_4Cl$	$CH_6N_3O_4Cl$
Molecular weight [g mol^{-1}]	159.54	159.54	159.54	159.54	159.54	159.54	159.54
Crystal system	Hexagonal	Hexagonal	Hexagonal	Hexagonal	Hexagonal	Hexagonal	Hexagonal
Space group	*R* 3 *m* (no. 160)	*R* 3 *m* (no. 160)	*R* 3 *m* (no. 160)	*R* 3 *m* (no. 160)	*R* 3 *m* (no. 160)	*R* 3 *m* (no. 160)	*R* 3 *m* (no. 160)
a [Å]	7.6180(4)	7.6428(15)	7.5595(6)	7.5534(4)	7.5310(4)	7.5123(4)	7.4965(3)
b [Å]	7.6180(4)	7.6428(15)	7.5595(6)	7.5534(4)	7.5310(4)	7.5123(4)	7.4965(3)
c [Å]	9.2280(7)	9.277(4)	8.7694(10)	8.6935(17)	8.4767(18)	8.3522(7)	8.2508(6)
α [°]	90	90	90	90	90	90	90
β [°]	90	90	90	90	90	90	90
γ [°]	120	120	120	120	120	120	120
V [Å^3]	463.83(5)	469.3(2)	434.00(7)	429.55(9)	416.36(9)	408.21(5)	401.55(4)
Z	3	3	3	3	3	3	3
ρ_{calc} [g cm^{-3}]	1.713	1.693	1.831	1.850	1.909	1.947	1.979
T [K]	350	375	295	295	295	295	295

[1] K. V. Titova, V. Y. Rosolovskii, *Zhurnal Neorganicheskoi Khimii,* **1965**, *10*, 446–450.
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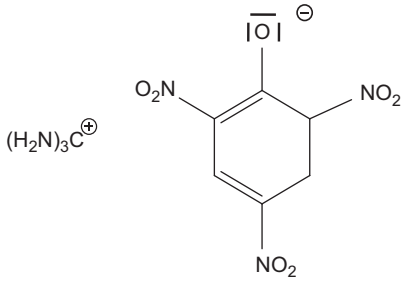
[6] Z. Pajak, M. Grottel, A. E. Koziol, *J. Chem. Soc. Faraday Trans. 2*, **1982**, *78*, 1529–1538.
[7] A. E. Koziol, *Z. Kristallographie*, **1984**, *168*, 313–315.
[8] M. Szafranski, *J. Phys. Chem. B*, **2011**, *115*, 8755–8762.
[9] M. Szafranski, *Cryst. Eng. Comm.*, **2014**, *16*, 6250–6256.
[10] 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**.
[11] T. Urbański, Ch. 20 in *Chemistry and Technology of Explosives*, *vol. II*, **1965**, Pergamon Press, Oxford.
[12] T. L. Davis, *The Chemistry of Powder and Explosives*, *vol. 2*, **1943**, John Wiley and Sons Inc., New York, p. 366.
[13] Y. N. Matyushin, *Estimation Method of Enthalpies of Formation of Salt Compounds*, ICT **2008**, Karlsruhe, Germany, pp. 44-1–44-15.
[14] J. J. Byrne, *Propellant Containing Guanidine Perchlorate-Lithium Perchlorate Eutectic in Homogeneous Phase with Polymeric Binder*, US Patent 3531338, 29th September **1970**.
[15] G. S. Pearson, *Perchlorates: A Review of Their Thermal Decomposition and Combustion, with an Appendix on Perchloric Acid*, R. P. E. Technical Report No. 68/11, Rocket Propulsion Establishment Westcott, Ministry of Technology, London, October **1968**.
[16] M. R. Udupa, *Propellants, Explosives, Pyrotechnics*, **1983**, *8*, 109–111.

Guanidinium picrate

Name [German, acronym]: Guanidine picrate [guanidinpikrat, GuPicr, GuP]
Main (potential) use: Can be used as a filler for armor-piercing shells
Structural formula:



	Guanidine picrate*	
Formula	$C_7H_8N_6O_7$	
Molecular mass [g mol^{-1}]	288.18	
Appearance at RT	Yellow, finely crystalline solid[5], yellow crystals[7]	
N [%]	29.16	
Ω(CO_2) [%]	−61.1	
$T_{m.p.}$ [°C]	>300[1], 310–333[4], 318.5–319.5 (with dec.)[5], >300 (melts with dec.)[7]	
$T_{dec.}$ [°C]	325[2], 280[4]	
ρ [g cm^{-3}]	sp. gr. = ~1.5[4]	
Heat of formation	−396.60 ± 2.47 kJ/mol ($\Delta H°_f$)[3], −1,376.22 ± 8.57 kJ/kg ($\Delta H°_f$)[3]	
	Calcd. (K-J)	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]		12,204.7 ± 8.4[3]
T_{ex} [K]		
$p_{C\text{-}J}$ [GPa]		
VoD [m s^{-1}]		6,500 (@ 1.50 g cm^{-3})[7] 6,500[4]
V_0 [L kg^{-1}]		

* Exists in two stereoisomeric forms: labile and stable (usually mixtures are formed)[8]

<table>
<tr><td>Initiating efficiency</td><td>Minimum initiating charge (g) of primary explosive compressed under 1,000 lb in^2 pressure required to detonate 0.4 g GuP: 0.30 g fulminate with reinforcing cap[6], 0.13 g HMTD with reinforcing cap[6], 0.15 g HMTD without reinforcing cap[6]</td></tr>
<tr><td>Solubility [g/mL]</td><td>Sparingly soluble in EtOH or H_2O (can be recrystallized from H_2O)[5]

Solubility, g/100 cc solvent[5]:

<table>
<tr><th>T (°C)</th><th>Water</th><th>EtOH</th><th>Acetone</th></tr>
<tr><td>0</td><td>0.005</td><td>0.077</td><td>0.455</td></tr>
<tr><td>10</td><td>0.038</td><td>0.093</td><td>0.525</td></tr>
<tr><td>20</td><td>0.070</td><td>0.122</td><td>0.605</td></tr>
<tr><td>30</td><td>0.100</td><td>0.153</td><td>0.695</td></tr>
<tr><td>40</td><td>0.150</td><td>0.200</td><td>0.798</td></tr>
<tr><td>50</td><td>0.230</td><td>0.255</td><td>0.920</td></tr>
<tr><td>60</td><td>0.350</td><td>0.321</td><td>1.075</td></tr>
<tr><td>70</td><td>0.480</td><td>0.413</td><td></td></tr>
<tr><td>80</td><td>0.700</td><td>0.548</td><td></td></tr>
<tr><td>90</td><td>1.010</td><td></td><td></td></tr>
<tr><td>100</td><td>1.380</td><td></td><td></td></tr>
</table></td></tr>
</table>

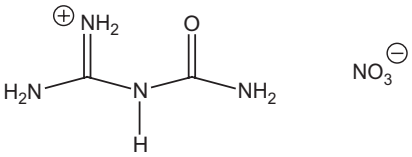
[1] J. P. Horwitz, C. C. Rila, *J. Am. Chem. Soc.*, **1958**, *80*, 431–437.
[2] C. Boyars, M. J. Kamlet, *Explosive Composition Containing Guanidinium Picrate*, US Patent 4,094,710 A, **1978**.
[3] T. S. Kon'kova, Y. N. Matyushin, *Russian Chemical Bulletin,* **1998**, *47*, 2387–2390.
[4] B. T. Fedoroff, O. E. Sheffield, *Encyclopedia of Explosives and Related Items*, *vol. 6*, US Army Research and Development Command, TACOM, Picatinny Arsenal, USA, **1974**.
[5] T. L. Davis, *The Chemistry of Powder and Explosives*, *vol. 1*, **1941**, John Wiley and Sons Inc., New York, pp. 168–169.
[6] T. L. Davis, *The Chemistry of Powder and Explosives*, *vol. 2*, **1943**, John Wiley and Sons Inc., New York, p. 452.
[7] J. Bebie, *Manual of Explosives, Military Pyrotechnics and Chemical Warfare Agents, Composition, Properties, Uses*, MacMillan Co., **1943**.
[8] V. v. Cordier, *Verh. d. Ges. Deutsch. Ntf. u. Aerzte*, **1904**, *II*, 105–108.

Guanylurea nitrate

Name [German, acronym]: Guanylurea nitrate, urea *N*-(aminoiminomethyl)-nitrate (1:1) [guanylurea-nitrat, guanylharnstoff-nitrat, GUN]

Main (potential) use: Possible substitute for nitroguanidine in propellants, possible component of gas-generant composition for automotive air bags[2]

Structural formula:



	Guanylurea nitrate		
Formula	$C_2H_7N_5O_4$		
Molecular mass [g mol^{-1}]	165.14		
Appearance at RT			
IS [J]	58 in (2 kg mass)[1], >40 (BAM)[4], >30 (BAM)[5]		
FS [N]	>360 (BAM)[4, 5]		
ESD [J]	Insensitive to Tesla coil V-24[4], insensitive (Tesla coil, ~20 kV)[5]		
N [%]	42.4		
Ω(CO_2) [%]	−33.91		
$T_{m.p.}$ [°C]	216 (crystals, dec.)[1], 203 (mpt. with dec., DSC @ 5 °C/min)[5]		
$T_{dec.}$ [°C]	216[2], 203 (DSC @ 5 °C/min)[4], 203 (mpt. with dec., DSC @ 5 °C/min)[5]		
ρ [g cm^{-3}]	1.54[1] 1.567 (pycnometry)[4]		
Heat of formation	−880 cal/g[2], −102.1 kcal/mol (ΔH_f)[3], −2,392 kJ/kg ($\Delta U°_f$)[4], −2,512 kJ/kg ($\Delta H_f°$, calcd., MP2)[4], −4,242 kJ/kg (ΔU_f, back calculated from ΔH_{comb} value)[5], −721 kJ/mol ($\Delta H°_f$)[5]		
Heat of combustion	−1,987 cal/g (ΔU_{comb})[4], −1,546 cal/g ($\Delta H_{comb.}$, exptl., bomb calorimetry)[5]		
	Calcd. (EXPLO5)	Lit. values	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]	927 cal/g (ΔH_{ex}, calcd., ICT code)[4]		364 cal/g[1]

T_{ex} [K]	2,624 (@ 1.567 g cm^{-3})[4] 1,577 (@ 1.567 g cm^{-3}, $\Delta U^{o}_{f} = -4{,}242$ kJ/kg)[5]		
$p_{C\text{-}J}$ [kbar]	17.4 GPa (@ 1.567 g cm^{-3})[4] 10.6 GPa (@ 1.567 g cm^{-3}, $\Delta U^{o}_{f} = -4{,}242$ kJ/kg)[5]		
VoD [m s^{-1}]	7,004 (@ 1.567 g cm^{-3})[4] 5,734 (@ 1.567 g cm^{-3}, $\Delta U^{o}_{f} = -4{,}242$ kJ/kg)[5]		
V_0 [L kg^{-1}]	858 (@ 1.567 g cm^{-3})[4] 849 (@ 1.567 g cm^{-3}, $\Delta U^{o}_{f} = -4{,}242$ kJ/kg)[5]		
I_{sp} [s]	177[4]		
Explosion T [°C]	320[1]		
100 °C heat test [% mass loss/h]	0.17/48[1]		
Vacuum stability test [cm^3/h]	1.54 mL per 5 g sample @ 120 °C in 40 h		
Solubility [g/mL]	Soluble in DMSO[5]		
Flame test	Burns (response to fast heating in flame test)[4], rapid burning with no explosion on being exposed to thermal shock in Bunsen flame[5]		

[1] S. M. Kaye, H. L. Herman, *Encyclopedia of Explosives and Related Items*, *vol. 10*, US Army Research and Development Command, TACOM, Picatinny Arsenal, USA, **1983**.

[2] I. V. Mendenhall, *Guanylurea Nitrate in Gas Generation*, US Patent 6,550,808 B1, April 22nd **2003**.

[3] D. D. Wagman, W. H. Evans, V. B. Parker, I. Halow, S. M. Baily, R. H. Schumm, *Selected Values of Chemical Thermodynamic Properties: Tables for the First Thirty-Four Elements in the Standard Order of Arrangement*, NBS Technical Note 270-3, U. S. Department of Commerce, National Bureau of Standards, Washington, USA, January **1968**.

[4] T. M. Klapötke, C. Sabate, *ZAAC*, **2010**, *636*, 163–175.

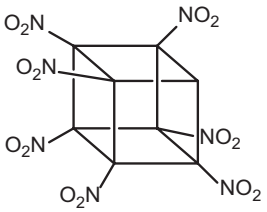
[5] T. M. Klapötke, C. M. Sabate, *Heteroatom Chem.*, **2008**, *19*, 301–306.

H

Heptanitrocubane

Name [German, acronym]: Heptanitrocubane [heptanitrocuban, HpNC]
Main (potential) use: Intermediate in the synthesis of octanitrocubane (ONC)[1], possible future powerful explosive and/or monopropellant[3]

Structural formula:



	Heptanitrocubane		
Formula	$C_8HN_7O_{14}$		
Molecular mass [g mol^{-1}]	419.14		
Appearance at room temperature (RT)	Colorless, solvent-free crystals obtained from diluting a soln. of HpNC in fuming nitric acid with sulfuric acid[2, 3]		
N [%]	23.39		
Ω(CO_2) [%]	−9.54		
$T_{dec.}$ [°C]	Well above 200[3]		
ρ [g cm^{-3}]	2.028[1], 2.028 (@ 21 °C, single crystal, X-ray)[2, 3]		
Heat of formation			
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]			
T_{ex} [K]			
$p_{C\text{-}J}$ [kbar]			
VoD [m s^{-1}]			
V_0 [L kg^{-1}]			
Solubility [g/mL]	Easily soluble in polar solvents, for example, acetone, THF, CH_2Cl_2[2], solns. in MeOH turn yellow[2]		

https://doi.org/10.1515/9783110672565-008

Compatibility	Solns. in MeOH turn yellow, however after addition of trifluoroacetic acid and evaporation of solvent non-decomposed HpNC was obtained[2], sensitive to base, can be deprotonated[2], NaF in MeOH catalyzed HpNC dec. as did amines such as 2,2,6,6-tetramethylpiperidine[2], powerful deflagration on addition of a microdrop of pyridine to dry HpNC solid[2]

	Heptanitrocubane[2]
Chemical formula	$C_8HN_7O_{14}$
Molecular weight [g mol^{-1}]	419.16
Crystal system	Orthorhombic
Space group	*Pbcn*
a [Å]	23.5942(13)
b [Å]	8.1735(7)
c [Å]	14.2642(5)
α [°]	90
β [°]	90
γ [°]	90
V [Å^3]	2,750.8(3)
Z	8
ρ_{calc} [g cm^{-3}]	2.028
T [K]	21 °C

Colorless, solvent-free crystals obtained from diluting a soln. of HpNC in fuming nitric acid with sulfuric acid[2]

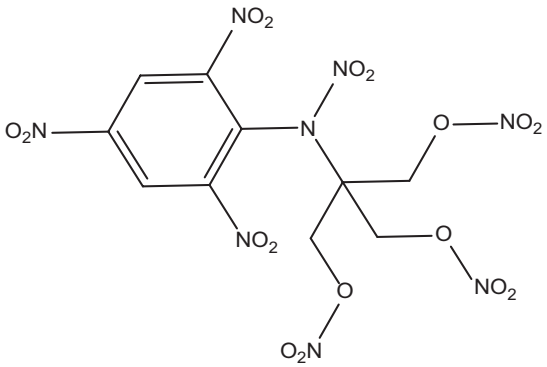
[1] J. P. Agrawal, R. D. Hodgson, *Organic Chemistry of Explosives*, John Wiley and Sons Ltd., **2007**, pp. 73–74.
[2] M.-X. Zhang, P. E. Eaton, R. Gilardi, *Angew. Chem. Int. Ed.*, **2000**, *39*, 401–404.
[3] P. E. Eaton, M.-X. Zhang, R. Gilardi, N. Gelber, S. Iyer, R. Surapaneni, *Propellants, Explosives, Pyrotechnics*, **2002**, *27*, 1–6.

Heptryl

Name [German, acronym]: Heptryl, *N*-(2,4,6 trinitrophenyl-*N*-nitramino)-trimethylolmethane trinitrate, *N*-(2,4,6-trinitrophenyl)-(tris-nitroxymethyl-methyl)-nitramine, *N*-nitro-*N*-picryl-trimethylol methyl-amine trinitrate

Main (potential) use:

Structural formula:



	Heptryl	
Formula	$C_{10}H_8N_8O_{17}$	
Molecular mass [g mol^{-1}]	512.21	
Appearance at RT		
IS [J]	Detonation of sample in tin foil when struck by hammer on an iron anvil but not if concrete anvil was used[4]	
N [%]	21.88	
$\Omega(CO_2)$ [%]	−21.9	
$T_{m.p.}$ [°C]	154–157 (dec.)[4], 154 (with dec.)[5]	
$T_{dec.}$ [°C]	154–157 (dec.)[4], ignites@ 180[4], explodes @ 360[4]	
ρ [g cm^{-3}]	1.924 ± 0.06 (@ 293.15 K)[1]	
Heat of formation	−405.0 kJ/kg (energy of formation)[2], 57.3 kcal mol^{-1} ($\Delta H°_f$)[4]	
Heat of combustion	1,160.7 kcal/mol (Q_c^V)[4]	
	Calcd. (K-J)	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]		9,480.5[2]
T_{ex} [K]		

$p_{C\text{-}J}$ [GPa]		
VoD [m s^{-1}]		
V_0 [L kg^{-1}]		787[2, 3]

Ballistic mortar test	143% TNT[4]
5 s explosion T [°C] Ignition T [°C]	180[4, 5] Does not explode <360[5]
Thermal stability	Exploded within 13 min in closed container @ 135 °C[4]

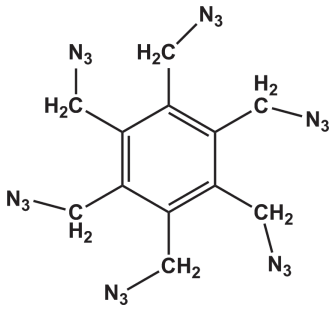
[1] Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© **1994–2017** ACD/Labs).
[2] R. Meyer, J. Köhler, A. Homburg, *Explosives*, 7th edn., Wiley-VCH, Weinheim, **2016**, p. 168.
[3] M. Jafari, M. Kamalvand, M. H. Keshavarz, A. Zamani, H. Fazeli, *Indian J. Engineering and Mater. Sci.,* **2015**, *22*, 701–706.
[4] B. T. Fedoroff, H. A. Aaronson, E. F. Reese, O. E. Sheffield, G. D. Clift, *Encyclopedia of Explosives and Related Items*, *vol. 1*, US Army Research and Development Command, TACOM, Picatinny Arsenal, USA, **1960**.
[5] *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**.

Hexakis(azidomethyl)benzene

Name [German, acronym]: Hexakis(azidomethyl)benzene [hexakis(azidomethyl) benzol, HAB]

Main (potential) use: Proposed as possible substitute for LA in less sensitive bridgewire detonators and as a substitute for tetrazene in percussion detonators[1, 2]

Structural formula:



	HAB
Formula	$C_{12}H_{12}N_{18}$
Molecular mass [g mol^{-1}]	408.35
Appearance at RT	White powder[2], light tan-colored solid[3]
IS [J]	$H_{50\%}$ = 1–2 in (ball drop, 7 g steel ball, 0.5 mm thick layer of HAB)[2], $H_{10\%}$ = 5 in (2 kg hammer, P.A.)[2], >120 in.oz (0.850 Nm) in M-42 primer cup-and-anvil assembly (120 in.oz is the max. attainable impact with the apparatus) and no increase in sensitivity on "sensitizing" HAB with 5% carborundum grit or 5% carborundum grit with 1% $KClO_4$)[2]
FS [N]	
ESD [J]	0.01 (minimum energy)
N [%]	61.8
Ω(CO_2) [%]	–117.55
$T_{m.p.}$ [°C]	162–165 (with dec., capillary mpt., uncorrected)[2], 164 (onset, endo, DTA @ 2.5 °C/min)[2], 165–168 (light tan colored solid)[3]
$T_{dec.}$ [°C]	162–165 (melts with dec., capillary method, uncorrected)[2], 186 (exo, onset), 212 (exo, peak max) (DTA @ 2.5 °C/min)[2]
ρ [g cm^{-3}]	1.460 (calcd., Cady's method)[2], 1.392 (pycnometry in 95% EtOH)[2], 1.222 (@ 16,000 psi/110 MPa)[2], 1.251 (@ 25,000 psi/172 MPa)[2]

<table>
<tr><td>Heat of formation</td><td colspan="3">438.4 kcal/mol ($\Delta H_f°$, calcd., using ΔH_c value determined in oxygen and $\rho = 1.460$ g cm^{-3})[2]</td></tr>
<tr><td>Heat of combustion</td><td colspan="3">–4,841.3 cal/g (measured, hot-wire ignition of HAB powder under 25 atm. oxygen pressure)[2], –1,171.4 cal/g (measured, hot-wire ignition of HAB powder in air)[2]</td></tr>
<tr><td></td><td>Calcd.
(EXPLO5 6.03)</td><td>lit. values</td><td>exptl.</td></tr>
<tr><td>$-\Delta_{ex}U°$ [kJ kg^{-1}]</td><td></td><td></td><td></td></tr>
<tr><td>T_{ex} [K]</td><td></td><td></td><td></td></tr>
<tr><td>$p_{C\text{-}J}$ [kbar]</td><td></td><td></td><td></td></tr>
<tr><td>VoD [m s^{-1}]</td><td></td><td></td><td>5,773 (@ 1.15 g/mL)[2]</td></tr>
<tr><td>V_0 [L kg^{-1}]</td><td></td><td></td><td></td></tr>
<tr><td>SSGT [cm]</td><td colspan="3">4.51 DB_g (@ 1.222 g/mL test density, @ 16,000 psi/110 MPa)[2]</td></tr>
<tr><td>5 s explosion T [°C]
1 s explosion T [°C]
Autoignition T [°C]</td><td colspan="3">255[2]
317[2]
173[2]</td></tr>
<tr><td>Thermal stability</td><td colspan="3">Thermally and hydrolytically stable[1]</td></tr>
<tr><td>Vacuum stability test [cm^3/h]</td><td colspan="3"><5 mL gas/5.0 g sample after 40 h @ 100 °C[2]</td></tr>
<tr><td>Burn rate [mm/s]</td><td colspan="3">Easy to ignite and did not detonate even at highest burning rates[2], extremely fast and extremely slow burning rates observed, probably due to lack of uniformity in pellet: 760.0[2], 0.01[2], 5.1[2], 790.0[2]</td></tr>
<tr><td>Solubility [g/mL]</td><td colspan="3">Data from[2]:
<table>
<tr><td>Solvent</td><td>g/100 mL solvent</td><td>T (°C)</td></tr>
<tr><td>Water</td><td>< 0.05</td><td>100</td></tr>
<tr><td>MeOH</td><td>< 0.05</td><td>65</td></tr>
<tr><td>Isopropanol</td><td>< 0.1</td><td>80</td></tr>
<tr><td>Toluene</td><td>2.0</td><td>95</td></tr>
<tr><td>Acetone</td><td>< 1.0</td><td>25</td></tr>
<tr><td>Acetone</td><td>12.3</td><td>56</td></tr>
<tr><td>Dioxane</td><td>< 1.0</td><td>25</td></tr>
<tr><td>Dioxane</td><td>16.0</td><td>95</td></tr>
<tr><td>THF</td><td>0.7</td><td>25</td></tr>
<tr><td>THF</td><td>5.3</td><td>67</td></tr>
<tr><td>DMF</td><td>34.0</td><td>85</td></tr>
</table>
NMR measured in $CDCl_3$ or DMSO[3]</td></tr>
</table>

Photosensitivity	Gradually darkens on exposure to sunlight and more rapid darkening on exposure to UV light[2]
Compatibility	Unaffected by stirring in distilled water for 168 h @ 60 °C[2], reacts violently with 96% sulfuric acid @ RT[2], dec. in 80% sulfuric acid @ RT[2], negligible reactivity @ 100 °C vacuum stability test in presence of Al 6061-T-6, stainless steel 303, low carbon steel or copper[2]
Laser sensitivity	Complete dec. in the beam of a pulsed tunable CO_2 laser (1 pulse, 28 J/cm^2, focused @ 9.75 µm), but no dec. occurred with unfocussed beam[2]
Stab sensitivity test	<2 in.ozf (inch ounce-force)/2.9 × 10^{-3} Nm (50% fire level, 25 mg HAB pressed into M-55 detonator cup @ 70,000 psi and backed with barium nitrate @ 10,000 psi)[2]
Minimum priming charge test	No dent in witness block using 100 mg loose HAB ignited by electric match[2], no dent in witness block using 100 mg HAB pressed @ 10 psi and ignited by electric match[2], no dent in witness block using 200 mg HAB pressed @ 10 psi and ignited by electric match[2], no dent in witness block using 300 mg HAB pressed @ 10 psi and ignited by electric match[2]

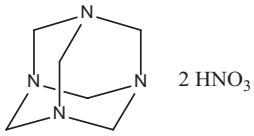
[1] J. P. Agrawal, *High Energy Materials: Propellants, Explosives and Pyrotechnics*, Wiley-VCH, **2010**, p. 134.
[2] E. E. Gilbert, W. E. Voreck, *Propellants, Explosives, Pyrotechnics*, **1989**, *14*, 19–23.
[3] J. V. Gavette, A. L. Sargent, W. E. Allen, *J. Org. Chem.*, **2008**, *73*, 3582–3584.

Hexamethylenetetramine dinitrate

Name [German, acronym]: Hexamethylenetetramine dinitrate, hexamine dinitrate [hexamethylentetramindinitrat]

Main (potential) use: Precursor for hexogen production by Bachmann process[1], not used as an explosive[5]

Structural formula:



	Hexamethylenetetramine dinitrate
Formula	$C_6H_{14}N_6O_6$
Molecular mass [g mol^{-1}]	266.21
Appearance at RT	
IS [J]	15 Nm[2]
FS [N]	240[2]
N [%]	31.57
$\Omega(CO_2)$ [%]	−78.1
$T_{m.p.}$ [°C]	170.5[3], 158[2], 160[5]
$T_{dec.}$ [°C]	174.0 (DSC @ 10 °C min^{-1})[3]
ρ [g cm^{-3}]	1.57[2]
Heat of formation	−382.9 kJ/mol ($\Delta H°_f$)[4], −1,438.3 kJ/kg ($\Delta H°_f$)[4], −1417.7 kJ/kg ($\Delta H°_f$)[2], −377.4 kJ/mol (enthalpy of form., exptl.)[6], −405.6 kJ/mol (enthalpy of form., calcd., emp.)[6], −382.9 kJ/mol (enthalpy of form., calcd., S-D method)[6], 96.70 kcal/mol ($-\Delta H_f$ (heat of form. @ standard conditions))[7]
Heat of combustion	Exptl. heat of combustion data[7]:

$-\Delta U_{B/M}$ (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)
3,571.93 ± 0.74	950.92	949.83	948.35

	Calcd. (EXPLO5 6.03)	Exptl.

$-\Delta_{ex}U°$ [kJ kg^{-1}]	3,528	2,642 [H_2O (l)][2] 2,434 [H_2O (g)][2]
T_{ex} [K]	2,407	
$p_{C\text{-}J}$ [GPa]	19.1	
VoD [m s^{-1}]	7,375 (@ TMD)	
V_0 [L kg^{-1}]	863	1,081[2]

Trauzl test [cm^3, % TNT]	220 cm^3 (10 g sample)[2]
Solubility [g/mL]	Soluble in water[2], insoluble in $CHCl_3$, Et_2O, EtOH, acetone[2]

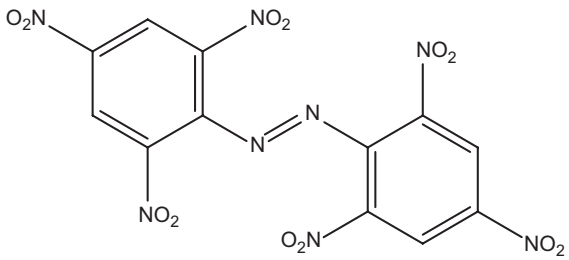
[1] W. E. Bachmann, J. C. Sheehan, *J. Am. Chem. Soc.*, **1949**, *71*, 1842–1845.
[2] R. Meyer, J. Köhler, A. Homburg, *Explosives*, 7th edn., Wiley-VCH, Weinheim, **2016**, pp. 169–170.
[3] H. Turhan, T. Atalar, N. Erdem, C. Özden, B. Din, N. Gül, E. Yildiz, L. Türker, *Propellants, Explosives, Pyrotechnics,* **2013**, *38*, 651–657.
[4] A. Salmon, D. Dalmazzone, *Journal of Physical and Chemical Reference Data*, **2007**, *36*, 19–58.
[5] T. Urbański, Ch. 19 in *Chemistry and Technology of Explosives*, *vol. II*, **1965**, Pergamon Press, Oxford.
[6] B. Nazari, M. H. Keshavarz, M. Hamadanian, S. Mosavi, A. R. Ghaedsharafi, H. R. Pouretedal, *Fluid Phase Equilibria,* **2016**, *408*, 248–258.
[7] 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**.

Hexanitroazobenzene

Name [German, acronym]: 2,2′,4,4′6,6′-Hexanitroazobenzene, bis(2,4,6)-trinitrophenyl diazine, hexanitroazobenzene [hexanitroazobenzol, HNAB]

Main (potential) use: Suggested for use in boosters and compound detonators[16]

Structural formula:



	Hexanitroazobenzene
Formula	$C_{12}H_4N_8O_{12}$
Molecular mass [g mol^{-1}]	452.21
Appearance at room temperature	Blood-red prisms if recryst. from nitrobenzene, glacial acetic acid or conc. nitric acid[7], orange crystals (if recrystallized from acetone)[16], orange[8]
IS [J]	9.07 (12 tool, 2.5 kg)[4], 7.85 (12B tool, 2.5 kg)[4], log $H_{50\%}$ = 1.57[5], 8.57[6], FI = 67% PA, 8.56 (1st reaction)[17], 7.85 (sound)[17], 32 cm (50% point, type 12 tool, 2.5 kg mass, sandpaper)[19]
ESD [J]	8.20[6], 8.2[22]
N [%]	24.78
Ω(CO_2) [%]	–49.5
$T_{phase\ transition}$ [°C]	Five polymorphs have been identified (hot-stage optical microscopy)[15]; HNAB-I and HNAB-III are stable from RT – 185 °C, HNAB-II is stable from RT – 205 °C[11, 15] HNAB-IV and HNAB-V are only formed in the melt during supercooling[11]. HNAB-II and HNAB-III transform rapidly through melt phase to HNAB-I[11], above 478 K solid – solid phase transitions occur; bulk HNAB (regardless of polymorphs present) melts at 496 K[14]
$T_{m.p.}$ [°C]	215–216[1, 7, 8], 220[4], 220–221[9, 18], 221–222[10], 223 (bulk samples regardless of polymorphic forms present)[11], 215[16]

$T_{dec.}$ [°C]	515 K (DTA onset)[17]		
ρ [g cm^{-3}]	2.15 ± 0.1 (@ 293.15 K)[2], 1.799 (phase I)[4], 1.750 (phase II)[4], 1.79[7], 1.775[20], 1.799 (TMD, obs., HNS-1)[8], 1.750 (TMD, obs., HNS-II)[8], 1.718 (TMD, obs., HNS-III)[8]		
Heat of formation	279 kJ/mol (EXPLO5 6.04 database), 535 kJ/kg (heat of form., $\Delta_f H$ @ 1 atm. and 298 K)[8], 241.8 kJ/mol (heat of form., $\Delta_f H$ @ 1 atm. and 298 K)[8], 58–67.9 kcal/mol[7], 67.9 kcal/mol ($\Delta_f H°$, exptl.)[20], +67.9 kcal/mol[21]		
Heat of combustion	$\Delta H°_c = -1{,}333.2$ kcal/mol[20]		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]	5,150	1.47 kcal/kg [H_2O (l)][8] 1.47 kcal/g [H_2O (l)][7] 1.42 kcal/g [H_2O (g)][8] 1.42 kcal/g [H_2O (g)][7]	1.47 kcal/g [H_2O (l)][7] 1.42 kcal/g [H_2O (g)][7]
T_{ex} [K]	3,875	3,900 (@ 1.60 g cm^{-3}, calcd. BKWR)[21] 4,620 (@ 1.60 g cm^{-3}, calcd. BKWS)[21]	
$p_{C\text{-}J}$ [GPa]	263	222 (@ 1.60 g cm^{-3}, calcd. BKWR)[21] 204 (@ 1.60 g cm^{-3}, calcd. BKWS)[21]	205[4] 205 (@ 1.60 g cm^{-3})[7, 21]
VoD [m s^{-1}]	7,838 (@ 1.799 g cm^{-3}, $\Delta_f H = 279$ kJ mol^{-1})	7,220 (@ 1.60 g cm^{-3}, calcd. BKWR)[21] 7,090 (@ 1.60 g cm^{-3}, calcd. BKWS)[21]	7,600–7,700 (0.1–0.3 in diameter column)[8] 7,250 (@ 1.77 g cm^{-3})[7] 7,311 (@ 1.60 g cm^{-3})[4, 13] 7,310 (@ 1.6 g cm^{-3})[3, 21]
V_0 [L kg^{-1}]	636		

<table>
<tr><td>Trauzl test [cm^3, % TNT]</td><td>123% TNT[7]</td></tr>
<tr><td>SSGT [cm]</td><td>6.38 mm (sensitivity, @ 1.774 g cm^{-3}, NSWC SSGT)[7], 12.04 mm (sensitivity, @ 1.383 g cm^{-3}, NSWC SSGT)[7], 5.6 mm (sensitivity, @ 1.601 g cm^{-3} pressed, LANL SSGT)[7]

Coarse-grade HNAB, lab sample under alcohol, IS: $H_{50\%}$ = 32 cm (2.5 kg mass, type 12 tool, sandpaper)[19]:

<table>
<tr><td rowspan="2">Loading pressure (kpsi)</td><td colspan="2">Density (g/cm^3)</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>8</td><td>1.476</td><td>0.0060</td><td>3.486</td><td>0.0142</td><td>0.0348</td><td>18</td></tr>
<tr><td>32</td><td>1.671</td><td>0.0051</td><td>4.848</td><td>0.0189</td><td>0.0318</td><td>12</td></tr>
<tr><td>64</td><td>1.766</td><td>0.0059</td><td>6.182</td><td>0.0611</td><td>0.0363</td><td>10</td></tr>
</table>

EBW (exploding bridgewire)-grade HNAB under EtOH/water[19]:

<table>
<tr><td rowspan="2">Loading pressure (kpsi)</td><td colspan="2">Density (g/cm^3)</td><td colspan="4">Sensitivity (DBG)</td><td rowspan="2">Remarks</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>1.383</td><td>0.0066</td><td>3.244</td><td>0.0051</td><td>0.0034</td><td>23</td><td></td></tr>
<tr><td>8</td><td>1.480</td><td>0.0039</td><td>3.251</td><td>–</td><td>–</td><td>23</td><td>No mixed response zone</td></tr>
<tr><td>16</td><td>1.582</td><td>0.0133</td><td>3.549</td><td>0.0554</td><td>0.0304</td><td>23</td><td></td></tr>
<tr><td>32</td><td>1.687</td><td>0.0030</td><td>4.382</td><td>0.0574</td><td>0.0502</td><td>23</td><td></td></tr>
<tr><td>64</td><td>1.774</td><td>0.0054</td><td>6.003</td><td>0.0512</td><td>0.0292</td><td>23</td><td></td></tr>
</table>
</td></tr>
<tr><td>Vacuum stability test [cm^3/h]</td><td>@ 200 °C (total cm^3 of gas evolved/no. of days): 0.4/2, 2.0/7, 9.8/14, 27.8/21[12], @ 175 °C (total cm^3 of gas evolved/no. of days): 0.1/2, 0.3/7, 0.6/14, 0.8/21, 0.9/28, 1.1/35, 1.2/42, 8,5/49, 9.2/56, 9.7/63, 10.6/70, 11.4/77, 12.5/84, 13.4/91[12], @ 150 °C (total cm^3 of gas evolved/no. of days): 0.1/2, 0.2/7, 0.2/14, 0.3/21, 0.3/28, 0.4/35, 0.4/42, 0.5/49, 0.5/56, 0.6/63, 0.6/70, 0.7/77, 0.7/84, 0.7/91[12]</td></tr>
</table>

<table>
<tr><td>Thermal stability</td><td>All values obtained by performing thin-layer chromatography on (s) to analyze how much undecomposed starting material remained[10]:
<table>
<tr><th>Time (min)</th><th>T (°C)</th><th>% Decomposition</th></tr>
<tr><td>720</td><td>230</td><td>14</td></tr>
<tr><td>4,380</td><td>230</td><td>100</td></tr>
<tr><td colspan="3"></td></tr>
<tr><td>342</td><td>245</td><td>32</td></tr>
<tr><td>540</td><td>245</td><td>44</td></tr>
<tr><td colspan="3"></td></tr>
<tr><td>61</td><td>260</td><td>15</td></tr>
<tr><td>130</td><td>260</td><td>23</td></tr>
<tr><td>187</td><td>260</td><td>42</td></tr>
<tr><td>240</td><td>260</td><td>68</td></tr>
<tr><td>288</td><td>260</td><td>73</td></tr>
<tr><td>360</td><td>260</td><td>100</td></tr>
<tr><td colspan="3"></td></tr>
<tr><td>30</td><td>280</td><td>10</td></tr>
<tr><td>60</td><td>280</td><td>49</td></tr>
<tr><td>92</td><td>280</td><td>60</td></tr>
<tr><td>118</td><td>280</td><td>100</td></tr>
</table></td></tr>
<tr><td>Vapor pressure [atm. @ °C]</td><td>1×10^{-7} mm Hg @ 100 °C[8]</td></tr>
<tr><td>Specific heat [cal/g/°C]</td><td>0.3[7, 20]</td></tr>
</table>

	HNAB-I[8, 11]	**HNAB-II**[8, 11]	**HNAB-III**[14]
Chemical formula	$C_{12}H_4N_8O_{12}$	$C_{12}H_4N_8O_{12}$	$C_{12}H_4N_8O_{12}$
Molecular weight [g mol^{-1}]	452.23	452.23	452.23
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1/c$ (no. 14)	$P2_1/a$	$P2_1$
a [Å]	10.149(4)	10.632(4)	15.4015(8)
b [Å]	8.263(3)	21.869(7)	5.5240(3)

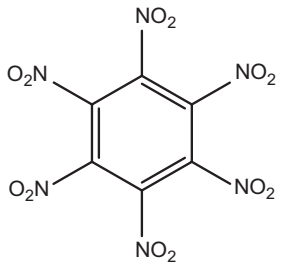
c [Å]	10.055(4)	7.585(3)	22.1182(11)
α [°]	90	90	90
β [°]	97.29(4)	102.56(4)	110.367(2)
γ [°]	90	90	90
V [Å^3]			1,764.13(16)
Z	2	4	4
ρ_{calc} [g cm^{-3}]	1.795	1.744	1.703
T [K]	23 °C	23 °C	298

[1] H. Leemann, E. Grandmougin, *Berichte der Deutschen Chemischen Gesellschaft*, **1908**, *41*, 1295–1305.
[2] Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© **1994–2017** ACD/Labs).
[3] M. H. Keshavarz, *Propellants, Explosives, Pyrotechnics*, **2008**, *33*, 448–453.
[4] B. M. Dobratz, P. C. Crawford, *LLNL Explosives Handbook – Properties of Chemical Explosives and Explosive Simulants*, Lawrence Livermore National Laboratory, January 31st **1985**.
[5] H. Nefati, J.-M. Cense, J.-J. Legendre, *J. Chem. Inf. Comput. Sci.*, **1996**, *36*, 804–810.
[6] N. Zohari, S. A. Seyed-Sadjadi, S. Marashi-Manesh, *Central Eur. J. Energ. Mater.*, **2016**, *13*, 427–443.
[7] *Military Explosives*, Department of the Army Technical Manual, TM 9-1300-214, Headquarters, Department of the Army, September **1984**.
[8] B. M. Dobratz, *Properties of Chemical Explosives and Explosive Simulants*, UCRL-5319, LLNL, December 15th **1972**.
[9] E. G. Kayser, *J. Energet. Mater.*, **1983**, *1:3*, 251–273.
[10] J. C. Hoffsommer, J. S. Feiffer, *Thermal Stabilities of Hexanitroazobenzene (HNAB) and Hexanitrobiphenyl (HNB)*, Naval Ordnance Laboratory, Maryland, USA, NOLTR 67–74, 23rd June **1967**.
[11] E. J. Graeber, B. Morosin, *Acta Cryst.*, **1974**, *B30*, 310–317.
[12] J. F. Baytos, *High-Temperature Vacuum Thermal Stability Tests of Explosives*, LA-5829-MS, LANL, January **1975**.
[13] J. R. Stine, *J. Energet. Mater.*, **1990**, *8*, 41–73.
[14] M. A. Rodriguez, C. F. Campona, A. D. Rae, E. Graeber, B. Morosin, *Acta Cryst.*, **2005**, *C61*, 0127.
[15] W. C. McCrone, *Crystallographic Study of Hexanitroazobenzene (HNAB)*,Sandia National Laboratories, Alberquerque, USA, **1967**.
[16] T. L. Davis, *The Chemistry of Powder and Explosives*, *vol. 1*, **1941**, John Wiley and Sons Inc., New York, pp. 189–190.
[17] S. Zeman, *Propellants, Explosives, Pyrotechnics*, **2003**, *28*, 308–313.
[18] E. G. Kayser, *Analysis Methods For Explosive Materials – I. Polynitro Compounds*, NSWC TR 81–123, Naval Surface Weapons Center, Maryland, USA, 3rd March **1962**.
[19] J. N. Ayres, L. J. Montesi, R. J Bauer, *Small Scale Gap Test (SSGT) Data Compilation: 1959–1972. Volume I. Unclassified Explosives*, AD-773 743, Naval Ordnance Laboratory, Maryland, USA, 26th October **1973**.
[20] P. E. Rouse, *J. Chem. Engineering Data*, **1976**, *21*, 16–20.
[21] M. L. Hobbs, M. R. Baer, *Calibrating the BKW-EOS with a Large Product Species Data Base and Measured C-J Properties*, in *Proceedings of the 10th International, Detonation Symposium, Office of Naval Research ONR 33395-12*, **1993**, pp. 409–418.
[22] L. Turker, *Electrostatic Discharge and Energetic Materials*, *To Chemistry Journal*, **2019**, *2*, 72–114.

Hexanitrobenzene

Name [German, acronym]: Hexanitrobenzene, [hexanitrobenzol, HNB]
Main (potential) use: Not stable enough for practical applications due to the fact that it decomposes in presence of moisture[9], practical use hindered by chemical instability[12]

Structural formula:



	Hexanitrobenzene		
Formula	$C_6N_6O_{12}$		
Molecular mass [g mol^{-1}]	348.10		
Appearance at RT	Yellow prism crystals on recryst. from $CHCl_3$[12]		
IS [J]	IS_{LL} = 0.3 m[1], $H_{50\%}$ = 11 cm (B.M., type 12 tool, 2.5 kg mass, 35 mg sample, garnet paper)[7], H_{50} = 11 cm (2.5 kg mass, type 12 tool)[14], A_{d1} = 100%, LL = 0.3 m [18], H_{50} = 15.6 ± 0.03 cm (type 12, ERL apparatus)[24], H_{50} = 16.8 ± 0.04 cm (type 12B, ERL apparatus)[24], H_{50} = 0.12 m[25], $H_{50\%}$ = 11 cm (2.5 kg mass, type 12 tool, 35 mg sample in conical pile, 1 in^2 garnet paper) [27], $H_{50\%}$ = 11 cm (2.5 kg mass)[28]		
N [%]	24.14		
$\Omega(CO_2)$ [%]	0		
$T_{m.p.}$ [°C]	246–262[5, 12, 21], 245–246 (recryst.)[17]		
$T_{dec.}$ [°C]			
ρ [g cm^{-3}]	1.965[13], 2.02 (@ TMD)[15], 1.99[19, 27]		
Heat of formation	47.5 kcal mol^{-1} (exptl.)[8], 420.7 kJ/kg (ΔH_f, ICT thermochemical database)[10], 1,57.0 kcal/kg (enthalpy of formation)[11], 15.7 kcal/mol (ΔH_f)[13], 65.69 kJ/mol[15], 39.7 kJ/mol (ΔH_f)[19], 10.0 kcal/mol[23], –36.4 kcal/mol (ΔH_f (g) @ 25 °C, calcd., MINDO/3)[26]		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.

<table>
<tr>
<td>$-\Delta_{ex}U°$ [kJ kg^{-1}]</td>
<td></td>
<td>1,620 kcal/kg (@ 1.640 g cm^{-3}, calcd.) [H_2O vapor][11]

$-\Delta H_{det}$ = 6.89 kJ/g[19]

Data from[20] (HNB ρ = 1.973 g/cm^3, $\Delta H_f°$ = 200.8 kJ/mol)[20]:

<table>
<tr><td>BKW-RDX</td><td>7.33</td></tr>
<tr><td>BKW-R</td><td>7.24</td></tr>
<tr><td>BKW-RR</td><td>7.18</td></tr>
<tr><td>[8]</td><td>7.36</td></tr>
<tr><td>[9]</td><td>6.88</td></tr>
<tr><td>[9]</td><td>7.36</td></tr>
</table>

Heat of explosion = 1,640 cal g^{-1} (@ 2.0 g cm^{-3})[22]</td>
<td>1,651 kcal/kg (@ 1.640 g cm^{-3}) [H_2O vapor][11]</td>
</tr>
<tr>
<td>T_{ex} [K]</td>
<td></td>
<td>5,183 (@ 2.0 g cm^{-3}, calcd.)[8]

4,509 (calcd., ICT code)[10]

7,203 (calcd., ICT code)[10]

4,942 (@ 1.965 g cm^{-3}, calcd., KLRR/C, THEOSTAR-T)[13]

5,297 (@ 1.965 g cm^{-3}, calcd., BKWC, THEOSTAR-T)[13]

4,422 (@ 1.965 g cm^{-3}, calcd., BKWR, THEOSTAR-T)[13]

HNB ρ = 1.973 g/cm^3, $\Delta H_f°$ = 200.8 kJ/mol, data from[20]:

<table>
<tr><td>BKW-RDX</td><td>3,244</td></tr>
<tr><td>BKW-R</td><td>4,631</td></tr>
<tr><td>BKW-RR</td><td>4,587</td></tr>
</table>

4,360 (@ 1.97 g cm^{-3}, calcd. BKWR)[23]

5,470 (@ 1.97 g cm^{-3}, calcd. BKWS)[23]</td>
<td></td>
</tr>
</table>

<table>
<tr>
<td>$p_{C\text{-}J}$ [kbar]</td>
<td></td>
<td>389 (@ 1.973 g cm^{-3}, calcd. emp.)[6]

473.6 (@ 2.0 g cm^{-3}, calcd.)[8]

128.3 MPa (calcd., ICT code)[10]

393 (@ 1.965 g cm^{-3}, calcd., KLRR/C, THEOSTAR-T)[13]

370 (@ 1.965 g cm^{-3}, calcd., BKWC, THEOSTAR-T)[13]

378 (@ 1.965 g cm^{-3}, calcd., BKWR, THEOSTAR-T)[13]

51.31 GPa (@ 2.07 g cm^{-3}, calcd., K-J)[16]

Data from[20] (HNB ρ = 1.973 g/cm^3, $\Delta H_f°$ = 200.8 kJ/mol; [‡] = calcd. by basic eqns. of hydrodynamic detonation model[20], values in GPa:

<table>
<tr><td>BKW-RDX</td><td>42.1</td></tr>
<tr><td>BKW-R</td><td>39.2</td></tr>
<tr><td>BKW-RR</td><td>37.7</td></tr>
<tr><td>single crystal $\rho_3 d_4^{20}$ of 2.00 g/cm^3</td><td>39.4</td></tr>
<tr><td>cited lit. values</td><td>40.9</td></tr>
<tr><td>cited lit. values</td><td>42.5</td></tr>
<tr><td>@ $Q_{calc} = Q_{max}$</td><td>35.6</td></tr>
<tr><td>Expt. ‡</td><td>40</td></tr>
</table>

44 GPa (@ 2.0 g cm^{-3})[22]

382 (@ 1.97 g cm^{-3}, calcd. BKWR)[23]

329 (@ 1.97 g cm^{-3}, calcd. BKWS)[23]

393 (@ 1.97 g cm^{-3}, calcd.)[27]</td>
<td>420 (@ 1.973 g cm^{-3})[6]

430 (@ 1.965 g cm^{-3})[13]</td>
</tr>
</table>

<table>
<tr>
<td>VoD [m s^{-1}]</td>
<td></td>
<td>9,110 (@ TMD (2.1 g cm^{-3}), calcd. R-P method)[4]

9,340 (@ 1.973 g cm^{-3}, calcd. emp.)[6]

9,630 (@ 2.0 g cm^{-3}, calcd.)[8]

9,410 (@ 1.965 g cm^{-3}, calcd., KLRR/C, THEOSTAR-T)[13]

9,160 (@ 1.965 g cm^{-3}, calcd., BKWC, THEOSTAR-T)[13]

8,830 (@ 1.965 g cm^{-3}, calcd., BKWR, THEOSTAR-T)[13]

10,330 (@ 2.07 g cm^{-3}, calcd-, K-J)[16]

HNB ρ = 1.973 g/cm^3, ΔH_f° = 200.8 kJ/mol[20] († = @ single crystal $\rho\, d^{20}{}_4$ of 2.00 g/cm^3; ‡ = calcd. by basic eqns. of hydrodynamic detonation model, § = @ $Q_{calc} = Q_{max}$), values in mm/µs[20]:

<table>
<tr><td>BKW-RDX</td><td>9.31</td></tr>
<tr><td>BKW-R</td><td>8.94</td></tr>
<tr><td>BKW-RR</td><td>8.76</td></tr>
<tr><td>†</td><td>9.11</td></tr>
<tr><td>cited lit. values</td><td>9.35</td></tr>
<tr><td>cited lit. values</td><td>9.40</td></tr>
<tr><td>§</td><td>8.48</td></tr>
<tr><td>Expt. ‡</td><td>~ 9.3</td></tr>
</table>

9,450 (@ 2.0 g cm^{-3})[22]

8,890 (@ 1.97 g cm^{-3}, calcd. BKWR)[23]

8,470 (@ 1.97 g cm^{-3}, calcd. BKWS)[23]

9,100 (@ 1.97 g cm^{-3}, calcd.)[27]</td>
<td>9,450 (@ 2.00 g cm^{-3})[3],

9,300 (@ 1.973 g cm^{-3})[6]

9,500 (@ 2.0 g cm^{-3})[8]

9,340 (@ 1.965 g cm^{-3})[13]

9,300 (@ 1.97 g cm^{-3}, calcd. BKWR)[23]</td>
</tr>
</table>

<table>
<tr><td>V_0 [L kg^{-1}]</td><td></td><td></td><td></td></tr>
<tr><td>I_{rel}</td><td></td><td>Data from[20] († = @ single crystal ρ $d^{20}{}_4$ of 2.00 g/cm^3; ‡ = calcd. by basic eqns. of hydrodynamic detonation model, § = @ $Q_{calc} = Q_{max}$)[20]:
<table><tr><td>BKW-RDX</td><td>129.9</td></tr><tr><td>BKW-R</td><td>126.0</td></tr><tr><td>BKW-RR</td><td>123.8</td></tr><tr><td>†</td><td>124.6</td></tr><tr><td>cited lit. values</td><td>125.9</td></tr><tr><td>cited lit. values</td><td>132.7</td></tr><tr><td>§</td><td>115.9</td></tr><tr><td>Expt. ‡</td><td>12.8</td></tr></table></td><td></td></tr>
<tr><td>Thermal stability</td><td colspan="3">Some lowering of mpt. and slight dec. on prolonged storage @ 25 °C[21]</td></tr>
<tr><td>Missile capacity</td><td colspan="3">105.5%[22]</td></tr>
<tr><td>Dipole moment, μ [D]</td><td colspan="3">0.07 (gas @ 25 °C, calcd., MINDO/3)[26], 0.01 (gas @ 25 °C, calcd., MNDO)[26]</td></tr>
</table>

Summary of experimental copper cylinder wall velocity data, PETN with a density of 1.763 g/cm^3 is the reference explosive, data from[15]:

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
1.965	19.05	1.950	1.700	1.880	1.955	18.8	21.6	19.3

Summary of code calculations with measure detonation velocities and detonation energies derived from JWL's[15]:

Initial density (g/cm^3)	PETN-adjusted BKWR Tiger, LLNL library, θ = 1850 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
1.965	–2	–2	0	–2	–5	–4	–11	–12	–10

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[15]:

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
1.918	−13.27	1.965	−13.59	−13.7	−13.8	−13.5	−13.1

JWL cylinder coefficients data from[15]:

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}
1.965	9.34	−13.20	43.0	1,047.883	7.982396	1.396122	4.472	0.85	0.28	2.986

	Hexanitrobenzene[2]
Chemical formula	$C_6N_6O_{12}$
Molecular weight [g mol^{-1}]	348.10
Crystal system	Monoclinic
Space group	*I*2/*c* (no. 15)
a [Å]	13.220(15)
b [Å]	9.130(40)
c [Å]	9.680(30)
α [°]	90
β [°]	95.50(50)
γ [°]	90
V [Å^3]	1,162.98
Z	4
ρ_{calc} [g cm^{-3}]	1.988
T [K]	295

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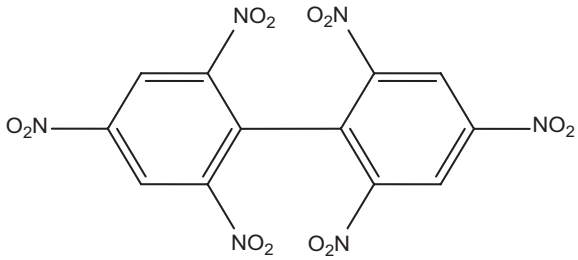
2,4,6,2′,4′,6′-Hexanitrobiphenyl

Name [German, acronym]: 2,4,6,2′,4′,6′-Hexanitrobiphenyl, hexa, 2,2′,4,4′,6,6′-hexanitro-1,1′-biphenyl, 2,4,6,2′,4′,6′-hexanitrodiphenyl, hexanitrodiphenyl [hexanitrobiphenyl, HNB*, HNBP, HNBPh]

Main (potential) use: Detonating composition component[26]

Structural formula:



* For HNB see also hexanitrobenzene

	2,4,6,2′,4′,6′-Hexanitrobiphenyl
Formula	$C_{12}H_4N_6O_{12}$
Molecular mass [g mol^{-1}]	424.19
Appearance at RT	Light yellow, thick crystals if recrystallized from toluene (contains half a molecule of toluene of crystallization)[19]
IS [J]	18.64[3], 2.79 (first reaction)[6, 21], 20.92 (sound)[6, 21], log $H_{50\%}$ = 1.93[7], 2.79 (Julius–Peters apparatus)[8], $H_{50\%}$ = 85 cm[9], $H_{50\%}$ = 70 cm (B.M., type 12 tool, 2.5 kg mass, 35 g sample, garnet paper)[10], 20.92 (Bruceton method)[18, 25], H_{50} = 70 cm (2.5 kg mass, type 12 tool)[23], log(H_{50}) = 1.929 (Kamlet/Adolph)[24], $H_{50\%}$ = 90 cm (2.5 kg mass, type 12 tool, ERL method)[27], $H_{50\%}$ = 70 cm (2.5 kg mass)[31] 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[30]:
ESD [J]	5.03[3–5, 32], 286.7 mJ[4]

Rotter impact data		US data	
F of I	Gas evolved (mL)	NSWC/NOL, ERL type 12	NWC B.M. Type 12
110	14.1	85	70

N [%]	19.81		
$\Omega(CO_2)$ [%]	−52.8		
$T_{phase\ transition}$ [°C]	128–130[15]		
$T_{m.p.}$ [°C]	263[1, 12, 19], 239.3–240.8[11], 238[12, 20], 242[12], 241–242[13], 239.3–240.8 (Thomas Hoover capillary melting point apparatus @ 2 °C/min)[22], 282 (DTA, exotherm, onset)[25]		
$T_{dec.}$ [K]	534 (DTA @ 5 °C/min)[6, 21], >320° (ignites)[12]		
ρ [g cm^{-3}]	1.6[1], 1.878 ± 0.06 (@ 293.15 K)[2], 1.74 (crystal)[14], ~1.61 (compressed under a pressure of 2,500 atm.)[20]		
Heat of formation	14.6 kcal/mol ($\Delta_f H°$, exptl.)[14]		
Heat of combustion	−1,279.9 kcal/mol ($\Delta H_c°$, exptl.)[14]		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]		4,654 MJ•kg^{-1} (Q_{real} @ TMD)[18, 25]	
T_{ex} [K]			
$p_{C\text{-}J}$ [GPa]		244[14]	
VoD [m s^{-1}]		7,500 (@ 1.74 g cm^{-3})[14] 7,480 (@ TMD, calcd., K-J)[18, 25]	7,100 (@ 1.60 g cm^{-3})[18, 25]
V_0 [L kg^{-1}]			

Critical T [K]	890 (explosion in 250 µs)[27]
Trauzl test [cm^3, % TNT]	360 cm^3[20], 344 cm^3[29]
SSGT [cm]	Recrystallized HNBP data from[28]:

Loading pressure (kpsi)	Density (g/cm^3)		Sensitivity (DBG)			
	Avg.	s	Avg.	g	s_m	N
8	1.248	Illegible	4.331	0.0470	0.0279	20
8	-	-	4.376	0.0013	0.0012	20
32	1.570	0.0148	5.080	0.0422	0.0276	20

5 s explosion T [°C] Ignition T [°C]	354[18, 25], >320[20]

<table>
<tr><td>Vacuum stability test [cm^3/h]</td><td>@ 200 °C, total vol. of gas evolved in cm^3/no. of days[17]: 0.6/2, 1.5/7, 2.2/14, 3.0/21, 3.6/28, 4.4/35, 4.8/42, 6.8/49, 7.6/56, 8.4/63, 9.1/70, 9.8/77, 10.9/84, 11.8/91[17]
@ 175 °C, total vol. of gas evolved in cm^3/no. of days[17]: 0.4/2, 0.6/7, 0.8/13, 1.1/21, 1.2/28, 1.4/35, 1.5/42, 1.7/49, 1.8/56, 2.0/63, 2.2/70, 2.4/77, 2.6/84, 2.8/91[17]
@ 150 °C, total vol. of gas evolved in cm^3/no. of days[17]: 0.2/2, 0.3/7, 0.3/14, 0.4/21, 0.4/28, 0.5/35, 0.5/42, 0.5/49, 0.6/56, 0.6/63, 0.7/70, 0.7/77, 0.8/84, 0.8/91[17]</td></tr>
<tr><td>Thermal stability</td><td>Values obtained by analyzing solid using thin-layer chromatography to analyze how much undecomposed sample remains[13]:
<table><tr><th>Time (min)</th><th>T (°C)</th><th>% Dec.[13]</th></tr><tr><td>1,305</td><td>230</td><td>5</td></tr><tr><td>7,222</td><td>230</td><td>9</td></tr><tr><td>1,934</td><td>250</td><td>38</td></tr><tr><td>168</td><td>280</td><td>36</td></tr><tr><td>295</td><td>280</td><td>54</td></tr><tr><td>389</td><td>280</td><td>96</td></tr></table>
0.9 cc/g/h gas evolved @ 260 °C[27]</td></tr>
<tr><td>Solubility [g/mL]</td><td>Insoluble in H_2O[19], slightly soluble in EtOH, acetone, benzene, toluene[19]</td></tr>
</table>

	Hexanitrobiphenyl[16]
Chemical formula	$C_{12}H_4N_6O_{12}$
Molecular weight [g mol^{-1}]	424.21
Crystal system	Triclinic
Space group	*P*-1 (no. 2)
a [Å]	8.1860(7)
b [Å]	12.1370(8)
c [Å]	16.2040(12)
α [°]	93.728(6)
β [°]	93.101(6)
γ [°]	104.688(6)

V [Å^3]	1,532.05
Z	4
ρ_{calc} [g cm^{-3}]	1.839
T [K]	150

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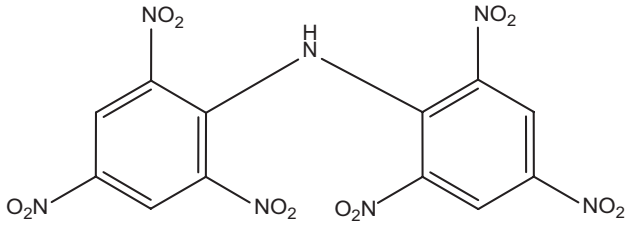
2,4,6,2′,4′,6′-Hexanitrodiphenylamine

Name [German, acronym]: Bis(2,4,6-trinitrophenyl) amine, 2,2′,4,4′,6,6′-hexanitrodiphenylamine, hexanitrodiphenylamine, dipicrylamine, 2,4,6-trinitro-*N*-(2,4,6-trinitrophenyl) benzenamine, 2,4,6,2′,4′,6′-hexanitrodiphenylamine, hexite, hexamite, hexil [hexanitrodiphenylamin, hexa, hexamin, hexyl, HNDPhA, HNDP, DPA]

Main (potential) use: Component of underwater explosives[1], component of fusible compositions with TNT (with or without ammonium nitrate) for filling torpedoes, bombs or marine mines in World War I and World War II[20], was used as component of hexanite[26], booster explosive[29], was used as booster and bursting charge in World War II[30]

Structural formula:



	HNDP
Formula	$C_{12}H_5N_7O_{12}$
Molecular mass [g mol^{-1}]	439.21
Appearance at RT	Yellow needles[20], small yellow needles[22], yellow – orange crystalline solid[26], yellow – brown solid as manufactured[26], yellow prisms from acetic acid or 93% nitric acid[28], yellow crystals[28, 29], yellow – brownish-yellow crystals[30], yellow crystalline powder[31], may be loose, dense, or finely crystalline depending on the production method[31], yellow prisms[33]
IS [J]	7.5 Nm[1], 11.77[5], 10.16 (1st reaction)[7, 13, 23], 11.81 (sound)[7, 23], H_{50} = 48 cm[12], $H_{50\%}$ = 48 cm[14], 35 cm (max. fall for $^0/_5$ shots, 2 kg mass, B.M.)[15], 9 in (2 kg mass, P.A.)[15], lower than that of tetryl, but higher than that of PA[20], 40 cm (2 kg mass, *Kast*)[20], 10 cm (10 kg mass, *Kast*)[20], slightly less sensitive than tetryl and tetranitroaniline[22], $H_{50\%}$ = 45 cm (5 kg mass, several decigrams sample, sample contained in small iron cup (0.2 mm thick) covered with 0.2 mm thick iron disk)[22], H_{50} = 48 cm (2.5 kg mass, type 12 tool)[25]

FS [N]	>353[1]		
ESD [J]	5.02[5, 6, 34]		
N [%]	22.32		
$\Omega(CO_2)$ [%]	−52.8		
$T_{m.p.}$ [°C]	233–235[2], 240–241[1], 245 (with dec.)[31], 243–245 (with dec.)[20, 26, 28], 243.0–244.5 (with dec.)[22], ~240[28], >238 (with dec.)[29, 33], 240–245[30], 238.5–239.5 (crude)[31]		
$T_{dec.}$ [K]	513 (DTA @ 5 °C min^{-1})[7, 23]		
ρ [g cm^{-3}]	1.64[1], 1.938 ± 0.06 (@ 293.15 K)[3], sp. gr. = 1.653 (crystal)[20] ρ under pressing[20]: 1.43 (@ <330 kg/cm^2)[20], 1.56 (@ <660 kg/cm^2)[20], 1.59 (@ <1,000 kg/cm^2)[20], 1.60 (@ <1,330 kg/cm^2)[20] ρ under pressing (pellets of HNDP mixed with 1% stearic acid)[22]: 1.43 (@ 5,000 lb/in^2)[22], 1.56 (@ 10,000 lb/in^2)[22], 1.59 (@ 15,000 lb/in^2)[22], 1.60 (@ 20,000 lb/in^2)[22]		
Heat of formation	50.9 kJ/mol (enthalpy of form., calcd., emp.)[4], 44.6 kJ/mol (enthalpy of form., exptl.)[4], -84.8 kJ/mol (enthalpy of form., calcd., S-D method)[4], −10.3 kcal/mol[15], 94.3 kJ/kg (enthalpy of form.)[1], −4.6 kcal/kg[20], −25.0 kcal/kg (enthalpy of form.)[24]		
Heat of combustion	1,314.1 kcal/mol[15]		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]	4,995	327.1–405.6 kcal/mol[15] 1,035 kcal/kg (*Kast*)[20] 1,054 kcal/kg (@ 1.700 g cm^{-3}, calcd.) [H_2O vapor][24]	4,075 [H_2O (l)][1, 9] 4,004 [H_2O (g)][1] 1,080 kcal/kg [H_2O (g)][11] 1,080 kcal/kg (@ 1.700 g cm^{-3}) [H_2O vapor][24] 1,035 cal/g (@ 1.67 g cm^{-3})[28] 1,080 kcal/kg[31]
T_{ex} [K]	3,574	3,450 °C (*Kast*)[20]	3,450 °C (@ 1.67 g cm^{-3})[28]
p_{C-J} [GPa]	29.6		

VoD [m s^{-1}]	8,207 (@ TMD)	6,898 (@ 1.58 g cm^{-3})[15, 22] 7,150 (@ 1.67 g cm^{-3})[15, 20, 22] 6,900 (@ 1.58 g cm^{-3})[20] 7,100 (@ 1.64 g cm^{-3}, *Kast*)[20] 6,995 (@ 1.58 g cm^{-3})[28] 7,145 (@ 1.67 g cm^{-3})[28]	7,200 (@ 1.60 g cm^{-3})[1] 7,200 (@ 1.64 g cm^{-3})[8] 7,400 (@ 1.64 g cm^{-3})[17] 22,600 ft/s (@ 1.6 g/mL)[26] 7,000 (@ 1.6 g cm^{-3})[28] 7,150 (@ 1.67 g cm^{-3})[28, 29] 6,900 (@ 1.58 g cm^{-3})[29] 7,145 (@ 1.60 g cm^{-3})[31]
V_0 [L kg^{-1}]	595	675 (Kast)[20]	791[1, 10] 675 (@ 0 °C and 760 mm Hg, @ 1.67 g cm^{-3})[28] 675[31]

Trauzl test [cm^3, % TNT]	320 cc (standard 10 g charge)[16], 102–108% TNT[17], 325–350 cm^3[20], 13.3 cc (small Trauzl test)[27] rel. strength cf. TNT = 1.09[27], 320 cc[28], 325 cm^3[32]
Sand test [g]	117–120% TNT[17], 0.5 g HNDP crushed 49.5 g sand cf. 48.0 g for TNT, that is, 103% TNT[15], 60.2 g (amount of sand crushed finer than 30 mesh, by total charge consisting of base charge of 0.50 g HNDP and 0.30 g priming charge of MF)[27], 48.5 g (amount of sand crushed finer than 30 mesh, by base charge of 0.50 g HNDP)[27], rel. strength cf. TNT = 1.11[27]
Ballistic mortar test	111–115% TNT[15, 17]
Initiation efficiency	0.18 g (minimum charge of fulminate–chlorate (90:10) necessary to completely detonate HNDP)[22, 31] Minimum initiating charge of primary explosive required for detonation (0.5 g charge HNDP in No. 8 detonator capsule with reinforcing cap, charges compressed under 3,400 lb/in^2 pressure)[21]: 0.165 g MF[21], 0.075 g DDNP[21], 0.05 g LA[21], no detonation resulted by DDNP if no reinforcing cap used[21]

	Minimum initiating charge of primary explosive required for detonation (0.4 g charge HNDP in detonator capsule, charges compressed under 1,000 lb/in^2 pressure)[21]: 0.05 g (HMTD)[21], 0.05 g (HMTD without reinforcing cap)[21], similar sensitivity to initiation as pentryl and tetryl[21] Minimum weight of priming charge which causes complete detonation of the base charge[27]: 0.075 g DDNP[27], 0.165 g MF[27], 0.005 g LA[27], can be detonated using detonators containing MF[28]
5 s explosion *T* [°C] Explosion *T* [°C] Initiation *T* [°C] Detonating *T* [°C]	 250 (heating rate @ 5 °C/min)[15], instantaneous explosion >360[15], 250–260[28] 250 (@ heating rate 2 °C/min)[20], 258 (heated from 100 °C @ 20 °C/min)[22], 250 (heated form 100 °C @ 5 °C/min)[22] ~237[26]
Thermal stability	Unchanged after heating for 30 days @ 95 °C[20], stable in storage at elevated temperatures[28], no dec. after heating for 3 h @ 40 °C[28], no dec. after heating for 3 h @ 160 °C[28], no dec. after heating for 3 h @ 180 °C[28]
Vacuum stability test [cm^3/h]	4.4 mL gas evolved from 5 g sample in 48 h @ 120 °C[15]
Burn rate [mm/s]	Burns underwater[26]
Solubility [g/mL]	Poorly soluble in most common organic solvents[20], soluble in hot acetic acid, nitrobenzene, acetone[20], insoluble in $CHCl_3$[22], soluble in EtOH, acetone[22], sparingly soluble in Et_2O[22], soluble in acetone, warm glacial acetic acid, nitric acid and aq. alkaline solutions (except aq. KOH)[26], almost insoluble in water or chloroform[28], slightly soluble in Et_2O or cold acetic acid[28], moderately soluble in EtOH[28], readily soluble in acetone, warm acetic acid or alkalies except aq. KOH[28], insoluble in water and common organic solvents[31], can be recryst. from acetone, glacial acetic acid and conc. nitric acid[31], insoluble in water, acetone, EtOH, Et_2O[33], soluble in alkalies, glacial acetic acid[33]
Hygroscopicity	Only slightly hygroscopic @ RT[20], 0.09% moisture absorbed when exposed to air saturated with water vapor[20], slightly hygroscopic[26], 0.09%[31]
Photosensitivity	Turns brown on exposure to sunlight[26, 31]
Flash point [°C]	250[31]
Kast brisance	4.9 mm[31]
Fugacity	320 cc[31]

	DPA[16]	DPA[18]	DPA[19]
Chemical formula	$C_{12}H_5N_7O_{12}$	$C_{12}H_5N_7O_{12}$	$C_{12}H_5N_7O_{12}$
Molecular weight [g mol^{-1}]			
Crystal system	Orthorhombic	Orthorhombic	Orthorhombic
Space group	$P2_12_12_1$ (no. 19)	$P2_12_12_1$ (no. 19)	$P2_12_12_1$ (no. 19)
a [Å]	11.692	11.72	7.3586(1)
b [Å]	18.991	19.84	11.6401(2)
c [Å]	7.381	7.37	18.7345(4)
α [°]	90	90	90
β [°]	90	90	90
γ [°]	90	90	90
V [Å^3]	1,638.9	1,713.71	1,604.7
Z		4	4
ρ_{calc} [g cm^{-3}]		1.702	1.818
T [K]	295	295	100

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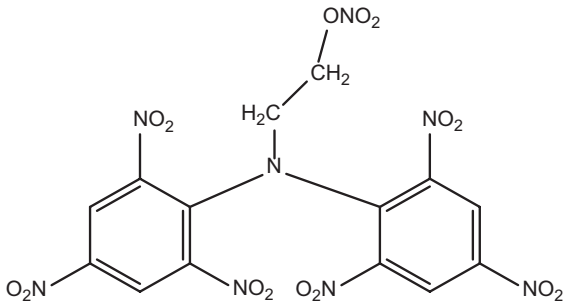
Hexanitrodiphenylaminoethyl nitrate

Name [German, acronym]: β(Hexanitrodiphenylamino)ethyl nitrate, 2-[bis(2,4,6-trinitrophenyl)amino-ethanol] nitrate, dipicrylamino-ethylol nitrate [hexanitrodiphenylaminoethylnitrat]

Main (potential) use: Suggested as base charge in compound detonators, possible uses as booster or component of reinforced detonators[5]

Structural formula:



	β(Hexanitrodiphenylamino)ethyl nitrate		
Formula	$C_{14}H_7N_8O_{15}$		
Molecular mass [g mol^{-1}]	528.26		
Appearance at RT	Pale-yellow glistening plates[3, 4], yellow crystals[5]		
IS [J]	35 cm (max. fall for $^0/_5$ shots, 2 kg mass)[1], 35 cm (max fall for $^0/_5$ explosions, 2,000 g weight, 0.02 g sample, BM small impact device)[4]		
FS [N]	No detonation when subjected to steel anvil and steel shoe, type B pendulum friction device, modification 1, 5 kg weight added to shoe[4]		
N [%]	21.21		
Ω(CO_2) [%]	−51.5		
$T_{m.p.}$ [°C]	184[−4]		
ρ [g cm^{-3}]	1.69[1], 1.27 (@ 3400 lb/sq.in)[1], 1.69 (true ρ)[4], 0.39 (apparent ρ when placed in cylinder and tapped)[4], 1.27 (pressed in detonator shell under reinforcing capsule under pressure of 239.0 kg/cm^2)[4], sp. gr. = 1.69[5]		
Heat of formation			
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]			
T_{ex} [K]			

$p_{C\text{-}J}$ [kbar]			
VoD [m s^{-1}]			
V_0 [L kg^{-1}]			
Trauzl test [cm^3, % TNT]	134% TNT[1], ~3% more effective than pentryl (small Trauzl test)[3], 16.3 (expansion of cavity in block, small Trauzl block)[4], rel. strength = 1.34 of TNT (small Trauzl block)[4]		
Sand test [g]	51.1 (0.5 g sample)/120% TNT[1], ~7% less effective than pentryl[3], 62.8 g (by total charge consisting of base charge of 0.50 g of test explosive and 0.30 g MF priming charge, no. 2 sand test bomb, sand crushed finer than 30 mesh, BM method)[4], 51.1 g (by base charge of 0.50 g of test explosive, no. 2 sand test bomb, sand crushed finer than 30 mesh, BM method)[4], rel. strength cf. TNT = 1.20[4]		
Initiation efficiency	Minimum detonating charge of primary explosive required to cause complete detonation: 0.05 g DDNP, 0.16 g MF, 0.04 g LA		
5 s explosion *T* [°C] Ignition *T* [°C]	390–400[1], 390–400 (if rapidly heated)[3–5] Using molten metal bath (chromel–alumel couple)[4]: instantaneously @ 450 °C[4], 0.25–0.5 s @ 440 °C[4], 0.5 s @ 430 °C[4], 1–1.5 s @ 420 °C[4], 1.5–2 s @ 400 °C[4], failed to ignite in 5 trials @ 390 °C[4]		
Thermal stability	Stored in the dry state for 6 months without discoloration or visible signs of dec.[4]		
100 °C heat test [% mass loss]	Slight discoloration but no mass loss after 48 h (international 100 °C heat test)[4]		
International 75 °C heat test	No discoloration or mass loss in 48 h @ 75 °C in international thermal stability test[1, 4]		
Solubility [g/mL]	Soluble in acetone[3, 4], very soluble in nitrobenzene, 1,4-dioxane, nitric acid, pyridine, aniline and hot ethylene glycol[4], less soluble in xylene, acetone and acetic anhydride[4], slightly soluble in EtOH, ethyl ether, ethylene dichloride, ethyl acetate, amyl acetate, MeOH and benzene[4]		
Compatibility	Stored in the dry state for 6 months without discoloration or visible signs of dec.[4]		

[1] B. T. Fedoroff, O. E. Sheffield, *Encyclopedia of Explosives and Related Items*, *vol. 5*, US Army Research and Development Command, TACOM, Picatinny Arsenal, USA, **1972**.

[2] R. Meyer, J. Köhler, A. Homburg, *Explosives*, 7th edn., Wiley-VCH, Weinheim, **2016**, p. 173.

[3] T. L. Davis, *The Chemistry of Powder and Explosives*, *vol. 2*, **1943**, John Wiley and Sons Inc., New York.

[4] L. R. V. Clark, *Industrial and Engineering Chemistry*, **1934**, *26*, 554–557.

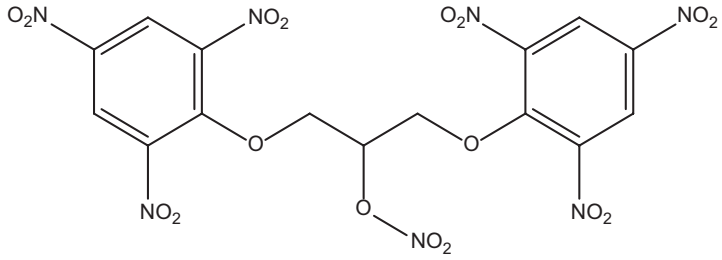
[5] J. Bebie, *Manual of Explosives, Military Pyrotechnics and Chemical Warfare Agents, Composition, Properties, Uses*, MacMillan Co., **1943**.

Hexanitrodiphenylglycerol mononitrate

Name [German, acronym]: Hexanitrodiphenylglycerol mononitrate
[heptanitrophenylglycerin]

Main (potential) use:

Structural formula:



	Hexanitrodiphenylglycerol mononitrate	
Formula	$C_{15}H_9N_7O_{17}$	
Molecular mass [g mol^{-1}]	559.27	
Appearance at room temperature		
IS [J]	23 Nm[1]	
N [%]	17.52	
$\Omega(CO_2)$ [%]	−50.1	
$T_{m.p.}$ [°C]	160–175[1]	
Heat of formation		
	Calcd. (K-J)	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]		
T_{ex} [K]		
$p_{C\text{-}J}$ [GPa]		
VoD [m s^{-1}]		
V_0 [L kg^{-1}]		

Critical diameter [cm]	
Trauzl test [cm^3, % TNT]	355[2]

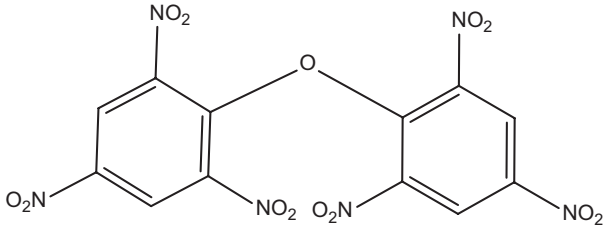
[1] R. Meyer, J. Köhler, A. Homburg, *Explosives*, 7th edn., Wiley-VCH, Weinheim, **2016**, pp. 173–174.
[2] M. Jafari, M. Kamalvand, M. H. Keshavarz, S. Farrashi, *ZAAC*, **2015**, *641*, 2446–2451.

2,4,6,2′,4′,6′-Hexanitrodiphenyl oxide

Name [German, acronym]: 2,4,6,2′,4′,6′-Hexanitrodiphenyl oxide, 2,4,6,2′,4′,6′-hexanitrodiphenyl ether, dipicrylether, dipicryloxide [hexanitrodiphenyloxid, HNDPO]

Main (potential) use: Detonating composition component[5]

Structural formula:



	2,4,6,2′,4′,6′-Hexanitrodiphenyl oxide	
Formula	$C_{12}H_4N_6O_{13}$	
Molecular mass [g mol^{-1}]	440.19	
Appearance at RT	White plates[5]	
IS [J]	8 Nm[1], does not detonate[4]	
N [%]	19.09	
Ω(CO_2) [%]	−47.3	
$T_{m.p.}$ [°C]	269[1, 5]	
ρ [g cm^{-3}]	1.70[1], 1.905 ± 0.06 (@ 293.15 K)[2]	
Heat of formation		
	Calcd. (K-J)	Exptl.
$-\Delta_{ex}U^o$ [kJ kg^{-1}]		
T_{ex} [K]		
$p_{C\text{-}J}$ [GPa]		
VoD [m s^{-1}]		7,180 (@ 1.65 g cm^{-3}, confined)[1] 7,180 (@ 1.70 g cm^{-3})[3]
V_0 [L kg^{-1}]		

Trauzl test [cm^3, % TNT]	373 cm^3[6]
Ballistic mortar test	63.6% of blasting gelatin[4]

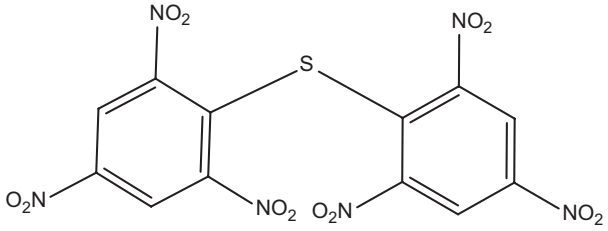
[1] R. Meyer, J. Köhler, A. Homburg, *Explosives*, 7th edn., Wiley-VCH, Weinheim, **2016**, p. 174.
[2] Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© **1994–2017** ACD/Labs).
[3] M. H. Keshavarz, *Propellants, Explosives, Pyrotechnics*, **2012**, *37*, 489–497.
[4] B. T. Fedoroff, O. E. Sheffield, *Encyclopedia of Explosives and Related Items*, *vol. 5*, US Army Research and Development Command, TACOM, Picatinny Arsenal, USA, **1972**.
[5] J. Bebie, *Manual of Explosives, Military Pyrotechnics and Chemical Warfare Agents, Composition, Properties, Uses*, MacMillan Co., **1943**.
[6] M. Jafari, M. Kamalvand, M. H. Keshavarz, S. Farrashi, *ZAAC*, **2015**, *641*, 2446–2451.

2,4,6,2′,4′,6′-Hexanitrodiphenylsulfide

Name [German, acronym]: 2,4,6,2′,4′,6′-Hexanitrodiphenylsulfide, bis(2,4,6-trinitrophenylsulfide, picryl sulfide, hexasulphide, hexide, 1,1′-thiobis(2,4,6-trinitrobenzene) [hexanitrodiphenylsulfid, dipicrylsulfid, DIPS, HNDPhS]

Main (potential) use: Used in explosive mixtures in World War I and World War II bombs[9], component in some bursting charges, proposed for use in reinforced detonators[15], used in World War I in drop bombs mixed with TNT[15], suggested for use to make closed spaces untenable due to SO_2 production on explosion[15]

Structural formula:



	2,4,6,2′,4′,6′-Hexanitrodiphenylsulfide
Formula	$C_{12}H_4N_6O_{12}S$
Molecular mass [g mol^{-1}]	456.25
Appearance at RT	Golden crystals[14], golden-yellow leaflets if recryst. from acetone[15], yellow crystals[17]
IS [J]	6 Nm[1], 7.30 (sound)[7], 2.94 (1st reaction)[7, 10, 16], 6.00 (sound)[7, 16], less sensitive than PA; FI = 83% PA[9], more sensitive than tetryl[9], $^0/_6$ shots = 36–39 cm (2 kg mass, Kast apparatus)[9], lower than that of tetryl, but higher than that of PA[14]
ESD [J]	2.54[5], 125.5 mJ[5], 2.56[6, 18]
N [%]	18.42
$\Omega(CO_2)$ [%]	−56
$T_{m.p.}$ [°C]	226[2], 234[1, 9, 14], 234 (golden-yellow leaflets recryst. from acetone)[15], 230–231[17]
$T_{dec.}$ [°C]	227–228[3], (detonates @ 320[9]), 525 K (DTA @ 5 °C/min)[7, 16]
ρ [g cm^{-3}]	1.65[1], 1.96 ± 0.1 (@ 293.15 K)[4], sp. gr. = 1.70 (@ 3,000 kg/sq cm)[9]

Heat of formation	14 kcal/mol[9]		
Heat of combustion	1,425 cal/mol (@ C^V)[9]		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]			3,682 [H_2O (g)][8]
T_{ex} [K]			
$p_{C\text{-}J}$ [GPa]			
VoD [m s^{-1}]			6,890 (@ 1.60 g cm^{-3})[11] 7,200 (@ 1.72 g cm^{-3})[11] 7,000 (@ 1.61 g cm^{-3}, confined)[1]
V_0 [L kg^{-1}]			

Trauzl test [cm^3, % TNT]	107% PA[9], 110%[12], 325 cc (10 g charge)[13], 325–350 cm^3[14], equal to or slightly larger than that of PA[14]
5 s explosion *T* [°C] Explosion *T* [°C] Initiation *T* [°C] Ignition *T* [°C]	 319 (@ heating rate of 20 °C/min)[9], 302 (@ heating rate of 5 °C/min)[9] 302–319 (depending on the rate of heating)[14] 319 (heated from 100 °C @ 20 °C/min)[15], 302 (heated from 100 °C @ 5 °C/min)[15], deflagrates @ 290[17]
Thermal stability	No dec. in 30 days heating (8 h per day) @ 95 °C[9], unchanged after 30 days @ 95 °C[14]
Solubility [g/mL]	Poorly soluble in most common organic solvents[14], sparingly soluble in EtOH, Et_2O[15], more soluble in acetone[15]

[1] R. Meyer, J. Köhler, A. Homburg, *Explosives*, 7th edn., Wiley-VCH, Weinheim, **2016**, pp. 174–175.
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[3] M. Pezold, R. S. Schreiber, R. L. Shriner, *J. Am. Chem. Soc.,* **1934**, *56*, 696–697.
[4] Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© **1994–2017** ACD/Labs).
[5] S. Zeman, J. Majzlík, *Central Europ. J. Energ. Mat.*, **2007**, *4*, 15–24.
[6] M. H. Keshavarz, Z. Keshavarz, *ZAAC*, **2016**, *642*, 335–342.
[7] S. Zeman, *Study of the Impact Reactivity of Polynitro Compounds Part IV. Allocation of Polynitro Compounds on the Basis of their Impact Sensitivities*, in *Proceedings of New Trends in Research of Energetic Materials*, NTREM 2002, April 24th–25th **2002**, pp. 434–443.
[8] W. C. Lothrop, G. R. Handrick, *Chem. Revs.*, **1949**, *44*, 419–445.
[9] B. T. Fedoroff, O. E. Sheffield, *Encyclopedia of Explosives and Related Items*, *vol. 5*, US Army Research and Development Command, TACOM, Picatinny Arsenal, USA, **1972**.
[10] S. Zeman, M. Krupka, *Propellants, Explosives, Pyrotechnics*, **2003**, *28*, 249–255.

[11] A. Smirnov, S. Smirnov, V. Balalaev, T. Pivina, *Calculation of Detonation Velocity and Pressure of Individual and Composite Explosives*, NTREM 17, 9th–11th April **2014**, pp. 24–37.
[12] 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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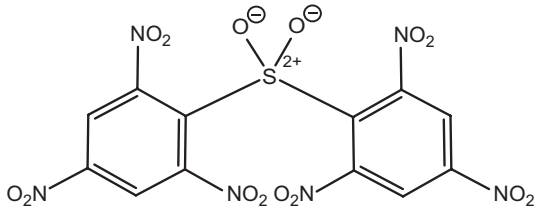
[18] L. Turker, *Electrostatic Discharge and Energetic Materials*, *To Chemistry Journal*, **2019**, *2*, 72–114.

2,4,6,2′,4′,6′-Hexanitrodiphenylsulfone

Name [German, acronym]: 1,3,5-Trinitro-2-[(2,4,6-trinitrophenyl)sulfonyl]-benzene, bis(2,4,6-trinitrophenyl) sulfone, 2,4,6,2′,4′,6′-hexanitrodiphenylsulfone, dipicrylsulfone, hexanitrodiphenylsulfone [hexanitrosulfobenzid, DIPSO, HNDPhSO]

Main (potential) use: Filling shells, bombs, torpedoes, used with TNT in aerial bombs in World War II[7], detonating composition component, used in mixtures with TNT and sometimes in mixtures with TNT and AN for filling bombs in World War I[11]

Structural formula:



	2,4,6,2′,4′,6′-Hexanitrodiphenylsulfone
Formula	$C_{12}H_4N_6O_{14}S$
Molecular mass [g mol^{-1}]	488.25
Appearance at room temperature	Yellow crystals[11], pale yellowish crystals[12]
IS [J]	3.86 (1st reaction)[6, 8, 13], 8.44 (sound)[6, 13], FI = 70% PA[7], max. fall for $^0/_6$ shots = 43 cm (2 kg mass, Kast apparatus)[7], similar to that of tetryl[11]
ESD [J]	10.24[4], 186.7 mJ[4], 10.54[5, 15]
N [%]	17.21
$\Omega(CO_2)$ [%]	−46
$T_{phase\ transition}$ [°C]	≥70 (as suspension, orthorhombic → monoclinic)[3], orthorhombic crystals formed @ 38 °C but above separation of solid from nitric acid >40 °C produces only monoclinic crystals[3]
$T_{m.p.}$ [°C]	307[1, 7, 12], 226[7], >254[7], 307 (dec.)[11], 307 (uncorrected, after recryst. from alcoholic acetone)[3], 338–345 (with dec., needle-like, orthorhombic crystals prepared from DIPS/CrO_3/nitric acid)[3], 335–345 (with dec., DIPSO prepared from novel method)[3]
$T_{dec.}$ [K]	530 (DTA)[6, 13], explodes @ 290 °C[7], 370[11]

ρ [g cm^{-3}]	1.962 ± 0.06 (@ 293.15 K)[2], 0.86 (bulk ρ, needle-like, orthorhombic crystals prepared from DIPS/CrO_3/nitric acid)[3], 1.1 (bulk ρ of DIPSO prepared from novel method)[3]	
Heat of formation		
	Calcd. (K-J)	Exptl.
$-\Delta_{ex}U^o$ [kJ kg^{-1}]		
T_{ex} [K]		
$p_{C\text{-}J}$ [GPa]		
VoD [m s^{-1}]		5,210 (@ 1.1 g cm^{-3})[3] 4,760 (1.2 grain per foot train of DIPS contained in metal sheath, DIPSO prepared from DIPS/CrO_3/nitric acid)[3] 5,210 (1.2 grain per foot train of DIPS contained in metal sheath, DIPSO prepared from novel method)[3]
V_0 [L kg^{-1}]		

Trauzl test [cm^3, % TNT]	115% TNT[9],107% PA[7]
Sand test [g]	70% PETN (DIPSO prepared from DIPS/CrO_3/nitric acid)[3]
5 s explosion T [°C] Explosion T [°C] Initiation T [°C] Ignition T [°C]	297 (@ heating rate of 5 °C/min)[7], 290[7] 297–308 (depending on heating rate)[11] 308 (heated form 100 °C @ 20 °C/min)[12], 297 (heated from 100 °C @ 5 °C/min)[12]
Thermal stability	No dec. after 30 days heating @ 95 °C (8 h per day)[7], long-term storage @ 130 °C showed no dec.[7], unchanged after heating @ 95 °C for 3 days[11], 3.5 h @ 450°F (DIPSO prepared from DIPS/CrO_3/nitric acid)[3], 7.5 h @ 450°F (DIPSO prepared from novel route)[3]
Vacuum stability test [cm^3/h]	@ 200 °C[10]: 2.4 cm^3 in 2 days[10] @ 175 °C[10]: 0.3/2 days, 0.7/7 days, 2.4/14 days, 7.1/21 days, 20.5/28 days[10] @ 150 °C[10, 14]: 0.1/2 days, 0.2/7 days, 0.2/14 days, 0.3/21 days, 0.3/28 days, 0.3/35 days, 0.4/42 days, 0.5/49 days, 0.5/56 days, 0.6/63 days, 0.7/70 days, 0.9/77 days, 1.1/84 days, 1.3/91 days[10, 14]
Solubility [g/mL]	Poor solubility in most common organic solvents[11]

	DIPSO[3]	**DIPSO**[3]
Chemical formula	$C_{12}H_4N_6O_{14}S$	$C_{12}H_4N_6O_{14}S$
Molecular weight [g mol^{-1}]		
Crystal system	Monoclinic	Orthorhombic
Space group	$C^5{}_{2h}$	$D^9{}_{2h}$
a [Å]	10.75	9.37
b [Å]	17.75	19.08
c [Å]	9.58	19.70
α [°]	90	90
β [°]	105.5	90
γ [°]	90	90
V [Å^3]		
Z	4	8
ρ_{calc} [g cm^{-3}]	1.841	1.84
T [K]		
	DIPSO prepared from novel method[3]	Needle-like crystals, DIPSO prepared using oxidation of DIPS using chromium trioxide and nitric acid[3]

[1] R. Meyer, J. Köhler, A. Homburg, *Explosives*, 7th edn., Wiley-VCH, Weinheim, **2016**, p. 174.

[2] Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© **1994–2017** ACD/Labs).

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[5] M. H. Keshavarz, Z. Keshavarz, *ZAAC*, **2016**, *642*, 335–342.

[6] S. Zeman, *Study of the Impact Reactivity of Polynitro Compounds Part IV. Allocation of Polynitro Compounds on the Basis of their Impact Sensitivities*, *Proceedings of New Trends in Research of Energetic Materials*, NTREM **2002**, April 24th–25th, pp. 434–443.

[7] B. T. Fedoroff, O. E. Sheffield, *Encyclopedia of Explosives and Related Items*, *vol. 5*, US Army Research and Development Command, TACOM, Picatinny Arsenal, USA, **1972**.

[8] S. Zeman, M. Krupka, *Propellants, Explosives, Pyrotechnics*, **2003**, *28*, 249–255.

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[11] T. Urbański, Ch. 16 in *Chemistry and Technology of Explosives*, *vol. 1*, **1964**, Pergamon Press, Oxford.

[12] T. L. Davis, *The Chemistry of Powder and Explosives*, *vol. 1*, **1941**, John Wiley and Sons Inc., New York, pp. 187–188.
[13] S. Zeman, *Propellants, Explosives, Pyrotechnics*, **2003**, *28*, 308–313.
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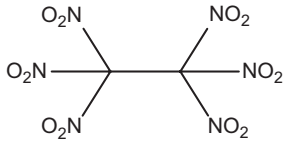
[15] L. Turker, *Electrostatic Discharge and Energetic Materials*, *To Chemistry Journal*, **2019**, *2*, 72–114.

Hexanitroethane

Name [German, acronym]: Hexanitroethane [hexanitroethan, HNE]
Main (potential) use: Oxidizer in propellants[1]
Structural formula:



	HNE		
Formula	$C_2N_6O_{12}$		
Molecular mass [g mol^{-1}]	300.05		
Appearance at room temperature	Colorless crystalline solid[20]		
IS [J]	4.7[2], comparable with PETN[14], often >1 m (2 kg hammer)[20]		
FS [N]	240[3]		
N [%]	28.01		
$\Omega(CO_2)$ [%]	+42.7		
$T_{m.p.}$ [°C]	150[1], 147[3], 142 (with partial dec. and sublimation)[14], 142 (with rapid dec.)[19], 142[20], 155 (with dec., recryst. material)[20], 150 (with dec.)[20]		
$T_{dec.}$ [°C]	136.61 (DSC @ 10 °C min^{-1})[4], 142 (melting with rapid dec.)[19]		
ρ [g cm^{-3}]	2.169 ± 0.06 (@ 293.15 K)[5], 2.248[8], 1.848 (cubic crystal @ 293 K)[11], 2.075 (monoclinic crystal, @ 145 K)[12], 1.85[3]		
Heat of formation	80.3 ± 0.4 kJ/mol[6], 267.7 ± 1.4 kJ/kg[6], 397.5 kJ/kg[8], 399.1 kJ/kg (enthalpy of form.)[3], 33.8 kcal/mol ($\Delta_fH°$ (g), exptl.)[17], −46.0 kcal/mol ($\Delta_fH°$ (g), calcd.)[17], 19.0 kcal/mol ($\Delta_fH°$ (cryst.))[17], 19.2 ± 0.1 kcal/mol ($\Delta_fH°$ (c))[15], 34.0 ± 0.2 kcal/mol ($\Delta_fH°$ (g))[15], 20.0 kcal/mol ($\Delta H_f°$)[16]		
$\Delta_cH°$ [kcal mol^{-1}]	−207.3 ± 0.1[15], −207.1[17]		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]	2,944	2,805.6 (calcd., K-J)[1] 750 cal/g[20]	3,021.7[1] 3,102[10] 2,884[3]

T_{ex} [K]	2,931	6,048 (calcd., K-J) [7] 2,440 (@ 1.86 g cm^{-3}, calcd.)[16]	
$p_{C\text{-}J}$ [GPa]	22.3	6.29 (calcd., K-J) [7] 235.5 kbar (@ 1.86 g cm^{-3}, calcd.)[16]	
VoD [m s^{-1}]	7,457 (@ 1.86 g cm^{-3}, $\Delta_f H = 83.7$ kJ mol^{-1})	4,907 (@ TMD) (calcd., K-J) [7] 7,540 (@ 1.86 g cm^{-3}, calcd.)[16]	4,950 (@ 0.91 g cm^{-3})[1] 7,580 (@ 1.86 g cm^{-3})[16]
V_0 [L kg^{-1}]	727		734[1, 3, 9] 672[10]

Trauzl test [cm^3, % TNT]	115% TNT[14], 117% TNT[20]
Ballistic mortar test	108% TNT[13, 14]
Thermal stability	Storable @ 25 °C but begins to dec. @ 75 °C and rapid dec. @ mpt. (142 °C)[19]
Enthalpy of vaporization [kcal mol^{-1}]	14.8 ± 0.1[15]
ΔH_{sub} [kJ/mol]	70.7 (exptl.)[18], 96.0 (calcd., QSPR)[18]

	HNE[11]	**HNE[11]**	**HNE[12]**
Chemical formula	$C_2N_6O_{12}$	$C_2N_6O_{12}$	$C_2N_6O_{12}$
Molecular weight [g mol^{-1}]	300.05	300.05	300.05
Crystal system	Orthorhombic	Cubic	Monoclinic
Space group	Not specified	*I*3	$P\,2_1/\,c$ (no. 14)
a [Å]	12.02	8.14(3)	10.152(2)
b [Å]	5.46	8.14(3)	9.311(2)
c [Å]	13.83	8.14(3)	10.251(2)
α [°]	90	90	90
β [°]	90	90	97.54(1)
γ [°]	90	90	90

V [Å^3]	907.652	539.353	960.6
Z	4	2	4
ρ_{calc} [g cm^{-3}]	Not given	1.848	2.075
T [K]	Not given	293	145

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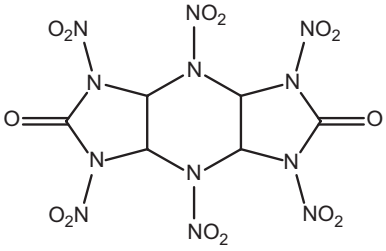
Hexanitrohexaazatricyclododecanedione

Name [German, acronym]: *Cis-syn-cis*-2,6-dioxo-1,3,4,5,7,8-hexanitrodecahydro-1*H*,5*H*-diimidazo[4,5-*b*:4′,5′-*e*]pyrazine, [HHTDD]

Main (potential) use: Potential submunition fill[1], (highest ρ reported for C, H, N, O explosive up to year 2002[2])

Structural formula:



	HHTDD		
Formula	$C_6H_4N_{12}O_{14}$		
Molecular mass [g mol^{-1}]	468.17		
Appearance at RT	Light-brown solid (crude product)[4], colorless solid after recryst. from $CH_3CN/CHCl_3$[4]		
N [%]	35.90		
$\Omega(CO_2)$ [%]	0		
$T_{m.p.}$ [°C]	215[1]		
$T_{dec.}$ [°C]	210 (explosively)[2, 4]		
ρ [g cm^{-3}]	2.07[1], 2.071[3]		
Heat of formation	−33.5 kJ/kg ($\Delta H_f°$)[3]		
	Calcd.(EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]		5,774 (Q_{cal}, calcd.)[3]	
T_{ex} [K]			
$p_{C\text{-}J}$ [kbar]		46.2 GPa[1] 42.5 GPa (@ 2.071 g cm^{-3}, calcd.)[3]	
VoD [m s^{-1}]		~9,750[1] 9,800 (@ 2.071 g cm^{-3}, calcd.)[3]	
V_0 [L kg^{-1}]			

<table>
<tr><td>LSGT [cm]</td><td>P_{cr} = 1.2 GPa (critical pressure of detonation initiation, calcd., LSGT)[3]</td></tr>
<tr><td>Thermal stability</td><td>Safe lifetime of ~55 years @ 20 °C[1]</td></tr>
<tr><td>Solubility [g/mL]</td><td>Recryst. from $CH_3CN/CHCl_3$, dry acetone/dry benzene[4], soluble in CH_3CN[4]</td></tr>
<tr><td>Compatibility</td><td>Dec. in humid air (85% RH) according to (t_{50} = 0.90 days)[1]:

<table>
<tr><td>Time (days)</td><td>R_t (%)</td></tr>
<tr><td>0</td><td>100</td></tr>
<tr><td>0.375</td><td>87.407</td></tr>
<tr><td>0.9375</td><td>51.424</td></tr>
<tr><td>1.458</td><td>13.679</td></tr>
<tr><td>2.354</td><td>0</td></tr>
<tr><td>4.792</td><td>0</td></tr>
</table>
Moist soil hydrolysis t_{50} = ~0.016 days (@ 23 °C, 25% wt. water/soil)[1]

Dec. in dry air (28% air RH) according to (t_{50} = 217 ± 15 days)[1]:

<table>
<tr><td>Time (days)</td><td>R_t (%)</td></tr>
<tr><td>0</td><td>100</td></tr>
<tr><td>5.858</td><td>99.277</td></tr>
<tr><td>33.800</td><td>98.174</td></tr>
<tr><td>47.035</td><td>94.759</td></tr>
<tr><td>60.975</td><td>91.615</td></tr>
<tr><td>74.778</td><td>93.573</td></tr>
<tr><td>125.808</td><td>84.492</td></tr>
</table>
Dec. in dry soil (28% air RH) according to (t_{50} = 294 ± 64 days)[1]:

<table>
<tr><td>Time (days)</td><td>R_t (%)</td></tr>
<tr><td>0</td><td>100</td></tr>
<tr><td>5.865</td><td>97.564</td></tr>
<tr><td>11.812</td><td>94.375</td></tr>
<tr><td>17.977</td><td>94.802</td></tr>
<tr><td>33.859</td><td>92.495</td></tr>
<tr><td>47.077</td><td>91.092</td></tr>
<tr><td>61.003</td><td>91.293</td></tr>
<tr><td>74.803</td><td>86.282</td></tr>
<tr><td>125.822</td><td>87.185</td></tr>
</table>
Easily decomposed by H_2O[2]</td></tr>
</table>

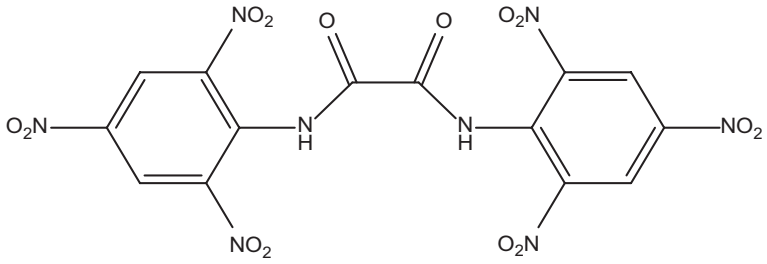
[1] R. D. Chapman, *Cyclic Dinitroureas as Self-Remediating Munition Charges*, SERDP project WP-1624, February **2009**.
[2] P. F. Pagoria, G. S. Lee, A. R. Mitchell, R. D. Schmidt, *Thermochim. Acta*, **2002**, *384*, 187–204.
[3] A. Smirnov, D. Lempert, T. Pivina, D. Khakimov, *Centr. Eur. J. Energet. Mater.*, **2011**, *8*, 233–247.
[4] M. Vedachalam, V. T. Ramakrishnan, J. H. Boyer, I. J. Dagley, K. A. Nelson, H. G. Adolph, R. Gilardi, C. George, J. L. Flippen-Anderson, *J. Org. Chem.*, **1991**, *56*, 3413–3419.

Hexanitrooxanilide

Name [German, acronym]: Hexanitrooxanilide, 2,2′,4,4′,6,6′-hexanitrooxanilide, [hexanitrodiphenyloxamid, HNO]

Main (potential) use: Pyrotechnic compositions[6], igniter powder[6], none because it undergoes hydrolysis readily[10]

Structural formula:



	HNO		
Formula	$C_{14}H_6N_8O_{14}$		
Molecular mass [g mol^{-1}]	510.24		
Appearance at RT	Almost white solid[13]		
IS [J]	14.22 (sound)[3], 8.70 (1st reaction)[5, 9, 12], 7.50 (sound)[5, 12], 15 in (P.A.)[7], 16 in (2 kg mass, confined, height of no detonation, P.A.)[14], 7.48 (15 in, 12 mg sample, 2 kg mass)[6]		
FS [N]	unaffected by steel shoe (friction pendulum test)[6], unaffected by fiber shoe (friction pendulum test)[6]		
ESD [J]	14.58[3, 15], 14.85[4]		
N [%]	21.96		
$\Omega(CO_2)$ [%]	−53.3		
$T_{m.p.}$ [°C]	295–300[1, 10, 11]		
$T_{dec.}$ [°C]	304[1], 302[6], 550 K (DTA @ 5 °C min^{-1})[5, 12]		
ρ [g cm^{-3}]	2.004 ± 0.06 (@ 293.15 K)[2]		
Heat of formation			
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]			
T_{ex} [K]			
$p_{C\text{-}J}$ [GPa]			

VoD [m s^{-1}]			5,100 (@ 0.90 g cm^{-3}, pressed product mixed with 2% dinitrotoluene)[10] 5,500 (@ 1.20 g cm^{-3}, pressed product mixed with 2% dinitrotoluene)[10] 6,800 (@ 1.47 g cm^{-3}, pressed product mixed with 2% dinitrotoluene)[10]
V_0 [L kg^{-1}]			

Trauzl test [cm^3, % TNT]	76% TNT[8]
Sand test [g]	134% TNT[8], 52.1 g (200 g bomb)[6]
Initiation efficiency	0.30 g LA minimum detonating charge[6], 0.25 g tetryl minimum detonating charge[6]
5 s explosion T [°C]	384[6, 7]
100 °C heat test [% mass loss]	0.07% mass loss in first 48 h[6, 7], 0.05% mass loss in second 48 h[6, 7], no explosion in 100 h[6, 7]
Vacuum stability test [cm^3/h]	0.40 cc/40 h @ 100 °C[6, 7]
Solubility [g/mL]	solubility values from[6]: Solvent / Solubility Nitrobenzene / < 3 g in 100 cc @ 23 °C, ~ 5 g in 100 cc @ 210 °C Water / 0.10 g in 100 cc @ 100 °C Ethyl alcohol / Insoluble Acetone / Insoluble Benzene / Insoluble Butyl acetate / Insoluble CCl_4 / Insoluble DMF / very soluble Et_2O / Insoluble Acetic acid / Insoluble Nitric acid / soluble Crystalline form / long rectangular glistening plates from nitrobenzene soluble in nitric acid[13], very soluble in DMF[13]
Hygroscopicity	0.19% @ 25 °C, 90% RH[6]

[1] R. Meyer, J. Köhler, A. Homburg, *Explosives*, 7th edn., Wiley-VCH, Weinheim, **2016**, p. 177.
[2] Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© **1994–2017** ACD/Labs).
[3] S. Zeman, *A Study of Chemical Micro-Mechanisms of Initiation of Organic Polynitro Compounds*, Ch. 2 in *Energetic Materials*, Part 2: Detonation, Combustion, P. A. Politzer, J. S. Murray (eds.), Theoretical and Computational Chemistry, Vol. 13, **2003**, Elsevier, pp. 25–60.
[4] M. H. Keshavarz, Z. Keshavarz, *ZAAC*, **2016**, *642*, 335–342.
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[6] *AMC Pamphlet Engineering Design Handbook: Explosive Series Properties of Explosives of Military Interest*, Headquarters, U.S. Army Materiel Command, January **1971**.
[7] S. M. Kaye, *Encyclopedia of Explosives and Related Items*, *vol. 8*, US Army Research and Development Command, TACOM, Picatinny Arsenal, USA, **1978**.
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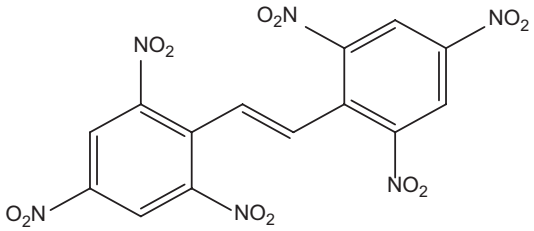
[9] S. Zeman, M. Krupka, *Propellants, Explosives, Pyrotechnics*, **2003**, *28*, 249–255.
[10] T. Urbański, Ch. 17 in *Chemistry and Technology of Explosives*, *vol. 1*, **1964**, Pergamon Press, Oxford.
[11] T. L. Davis, *The Chemistry of Powder and Explosives*, *vol. 1*, **1941**, John Wiley and Sons Inc., New York, p. 188.
[12] S. Zeman, *Propellants, Explosives, Pyrotechnics*, **2003**, *28*, 308–313.
[13] *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**.
[14] H. W. Voigt, *Impact Resistant Pressable Explosive Composition of High Energetic Material Content*, US Patent 4,251,301, February 17th **1981**.
[15] L. Turker, *Electrostatic Discharge and Energetic Materials*, *To Chemistry Journal*, **2019**, *2*, 72–114.

Hexanitrostilbene

Name [German, acronym]: 2,2′,4,4′6,6′-Hexanitrostilbene, hexanitrostilbene, 1,2-bis-(2,4,6-trinitrophenyl) ethylene, hexanitrodiphenylethylene, 1,1′-(1,2-ethenediyl)bis-(2,4,6-trinitrobenzene) [HNS]*

Main (potential) use: Secondary (high) explosive, thermostable, heat-resistant explosive, perforating the source rocks in gas and petroleum wells[38], space applications (e.g., stage operation on Apollo programme)[47], detonating fuses[47], HNS-I and HNS-II used in detonating fuses[47], HNS-IV used as initiator[47], booster explosives[47, 57], heat-resistant booster explosive[21], PBXs[21], mild detonating fuse end couplers[21], boosters[21]

Structural formula:



* HNS is available in four grades[39]:

- HNS-I: obtained from reaction of TNT with aq. NaOCl in THF/MeOH, purity = ≥98.5%, main impurity usually DPE (dipicrylethane)[39]
- HNS-II: obtained from recryst. of HNS-I, therefore usually much purer than HNS-I[39]
- HNS-FP: corresponds to HNS-fine particle, formed from crash precipitation of a DMF soln. of HNS into H_2O; contains 0.5–1.0% DMF solvent trapped in the particles which can be removed by washing with dioxane followed by MeOH; surface area usually 6 m^2/g[39]
- HNS-IV: crash precipitated material with surface areas of 10–15 ms/g, solvent concentration of up to 0.5% DMF possible[39]
- HNS-I: very fine crystalline substance purified by extraction of impurities[47], thin fluffy plates[47]
- HNS-II: obtained by recryst. of HNS-I, larger particle size, high bulk density, free-flowing solid cf. HNS-I[47], orthorhombic crystals[47]
- HNS-IV: superfine particles, surface area = 5.0–25.0 m^2/g[47], crash precipitated from HNS-II, HNS-II must be prior recryst. from DMF[47]
- HNS-IIA: refers to HNS material which has been recrystallized to a controlled bulk density (0.55 g/cm^3) from a mixed solvent refluxed over HNS-I[62]

	HNS
Formula	$C_{14}H_6N_6O_{12}$
Molecular mass [g mol^{-1}]	450.23
Appearance at RT	Yellow needles on recryst. from nitrobenzene[21], yellow solid[44], tan-yellow crystalline solid, exact color varies with particle size[49], pale-yellow needles[57], grade I HNS: light tan powder with small particle size and low ρ[58]
IS [J]	5 (<100 µm), 11.50[1], 3.64 (1st reaction)[3, 34], 11.50 (sound)[3, 34], 13.24 (ERL, HNS-I)[7, 8], 10.79 (ERL, HNS-I)[7, 8], 13.24 (ERL, HNS-II)[7, 8], 15.56 (ERL, HNS-II)[7, 8], $H_{50\%}$ = 44 cm (NOL-ERL apparatus, type 12 tool, 510 sandpaper, 2.5 kg mass, HNS-I)[12, 47], $H_{50\%}$ = 61 cm (NOL-ERL apparatus, type 12 tool, 510 sandpaper, 2.5 kg mass, HNS-II)[12, 47], 5 Nm[17], H_{50} = 1.13[19], IS_{LL} = 0.7 m[20], IS_{A50} = 2.0 m[20], 44 cm (HNS-I)[12], 61 cm (HNS-III)[12], H_{50} >112.2 cm[30], 5.0 Nm ($d_{50.3}$ = 13.7 µm)[42], 5.0 Nm ($d_{50.3}$ = 0.34 µm, ball milled)[42], H_{50} = 22 cm (5 kg mass)[43], H_{50} = 39 cm (2.5 kg mass, type 12 tool)[46], 44 cm (HNS-I, NOL apparatus)[21], 61 cm (HNS-II, NOL apparatus)[21], 47 cm (50% point, type 12 tool, 2.5 kg mass, sandpaper, HNS-I, dried for 24 h @ 150 °C in air oven, particle size: 99.7% through 325 mesh)[55], 55 cm (50% point, type 12 tool, 2.5 kg mass, sandpaper, HNS-I)[55], 61 cm (50% point, type 12 tool, 2.5 kg mass, sandpaper, HNS-II)[55], 39 cm (ERL machine, cf. tetryl = 32 cm)[57], 40 cm (type 12 tool, ERL machine, grade I, cf. tetryl = 32 cm)[58], 45 cm (type 12 tool, ERL machine, recryst. from nitrobenzene, cf. tetryl = 32 cm)[58], 61 cm (type 12 tool, ERL machine, grade II, cf. tetryl = 32 cm)[58], 9.7 (micro-HNS)[59], 12.4 (nano-HNS)[59], 45 cm (type 12 tool, 2.5 kg mass, ERL machine)[61] 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[64]:

HNS type	Rotter impact data		US data
	F of I	Gas evolved (mL)	NSWC/NOL, ERL type 12
I	90	7	54
II	90	12	

FS [N]	>360 (<100 µm), 440 kg/cm ($^{10}/_{10}$ no fires, HNS-I, HNS-II)[12], >240[17], 440 kg/cm (HNS-I)[21], 440 kg/cm (HNS-II)[21], F_{50} = 28.8 kgf ($^{1}/_{6}$)[19], 440 kg per cm (HNS-I and HNS-II)[21], $P_{fr.LL}$ = 200 MPa[20], $P_{fr.50\%}$ = 350 MPa[20], P = 28%[30], 240 ($d_{50.3}$ = 13.7 µm)[42], 192 ($d_{50.3}$ = 0.34 µm, ball milled)[42], 28% (raw HNS)[43]
ESD [J]	1.0 (<100 µm), 6.62[1], 5.32[2, 65], fires above 0.001 µfd (@ 8 kv, HNS-I)[12, 21], fires above 0.0001 µfd (@ 17 kv, HNS-II)[12, 21], $E_{50\%}$ = 7.040 (@ 293 K)[19], $E_{50\%}$ = 5.947 (@ 333 K)[19], $E_{50\%}$ = 0.66 ± 0.04 (Bruceton method)[32], E_{50} = 1.11[43]
N [%]	18.67
$\Omega(CO_2)$ [%]	−67.52
$T_{m.p.}$ [°C]	317[49], 315 (HNS-I)[7], 325 (HNS-I)[7], 316 (HNS-I)[12, 21, 22], 318 (HNS-II)[7, 22], 325 (HNS-II)[7], 319 (dec., HNS-II)[12, 21], 321 (sample in sealed cell)[19], 316 (dec. and explosions occur @ mpt.)[21], 320.4 (DSC)[30], 211 (no dec.)[31], 316 (dec., HNS-I, Thomas Hoover capillary melting point apparatus @ 2 °C/min)[36], 318 (dec., HNS-II, Thomas Hoover capillary melting point apparatus @ 2 °C/min)[36], 316–321 (lit. values)[38], 320 (DSC @ all heating rates from 2.5–20 °C/min)[38], 319.8 (DSC, T_{max}, synthesized HNS, d_{50} = 50 µm)[40], 320.7 (DSC, T_{max}, purified HNS, d_{50} = 300 µm)[40], 320.0 (DSC, T_{max}, HNS prepared by SDP (spray drying process), d_{50} = 3 µm)[40], 319.8 (DSC, raw HNS)[43], 315–316[44], 315–320 (DTA, standard sample)[44], 315–316 (dec.)[44], 319 (aged sample)[44], 316 (dec., crystals, recryst. from nitrobenzene, microscope hot stage)[57], 312–314 (dec., grade I)[58], 314–316 (dec., recryst. from nitrobenzene)[58], 318–319 (dec., grade II)[58], 322 (HNS-IIA, DTA/TGA)[62], 323 (HNS-IIA after undergoing two sterilization cycles @ 125 °C for 64 h each, DTA/TGA)[62]
$T_{dec.}$ [°C]	320 (DSC @ 5 °C/min), 544 K (DTA)[3, 34], 315 (HNS-I)[7, 12], 325 (HNS-II)[7, 12], 315 (exo, onset, DTA, HNS-I)[21], 325 (exo, onset, DTA, HNS-II)[21], 316[57], 344 (HNS-IIA, DTA/TGA)[62], 342 (HNS-IIA after undergoing two sterilization cycles @ 125 °C for 64 h each, DTA/TGA)[62] @ 8 °C min: T_{idb} = 323.9, T_w = 324.0, T_{max} = 328.9[24] @ 16 °C min: T_{idb} = 328.2, T_w = 345.0, T_{max} = 351.1[24] T_{cr} = 320–321[24] 349.9 (DSC, T_{max}, synthesized HNS, d_{50} = 50 µm)[40], 349.4 (DSC, T_{max}, purified HNS, d_{50} = 300 µm)[40], 343.7 (DSC, T_{max}, HNS prepared by SDP (spray drying process), d_{50} = 3 µm)[40], 317.9 (onset), 342.3 (peak max) (TGA, ultrafine spherical HNS)[40], 350.1 (TG-DSC, raw HNS)[43], ~304 (dec. onset, aged sample, T_{db}, TGA)[44], 333 (intensive dec. onset, T_{idb}, aged sample, TGA)[44], 330–335 (intensive dec. onset, T_{idb}, standard sample, DTA)[44], 312–314 (mpt. with dec., grade I)[58], 314–316 (mpt. with dec., recryst. from nitrobenzene)[58], 318–319 (mpt. with dec., grade II)[58]

ρ [g cm^{-3}]	1.718 (@ 150 K), 0.32–0.45 (bulk HNS-I)[12, 47], 0.45–1.0 (bulk, HNS-II)[12, 47], 1.681 (@ 298 K, calcd.), 1.740 (@ TMD)[9], 1.74 (@ TMD)[17, 44], 1.74 (@ TMD)[51], 1.740 (HNS-type I, TMD)[21], 1.740 (crystal)[23, 47], 1.72 (nominal)[21, 44], 1.601 ± 0.007 (SPD HNS pellets of height 0.203 ± 0.004 cm, using an Instron)[45], 1.74 @ 25 °C[47], 1.740 (crystal, flotation method)[57], 0.25–0.30 (bulk ρ of Grade I powder)[58], 0.20–0.25 (bulk ρ of thin needles obtained on recryst.)[58], 0.4–0.62 (bulk ρ, grade II)[58], 0.25 (bulk ρ, HNS-I)[58], 0.24 (bulk ρ, recryst. from nitrobenzene)[58], 0.55 (bulk ρ, grade II)[58]		
Heat of formation	58.1 (ΔH_f, @ 1 atm. and 298 K)[13], 173.8 kJ/kg (enthalpy of form.)[17], –13.89 kcal/mol (enthalpy of form., (s))[47], 129 kJ/kg (ΔH_f, @ 1 atm and 298 K)[13], 41.5 kcal/kg (ΔH_f)[19], 18.7 kcal/mol (enthalpy of form.)[44], 13.9–18.7 kcal/mol[21], 78.24 kJ/mol[51]		
Heat of combustion	3,451 cal/g (HNS-I)[12, 21], 3,451 cal/g (HNS-II)[12, 21], enthalpy of comb. = –1,535.34 ± 1.08 kcal/mol[47]		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]	4,612	1,428.4 J/g (@ 1.82 g cm^{-3}, calcd., K-J)[28] 142 kcal/g [H_2O (l)][13] 136 kcal/g [H_2O (g)][13] 1,058 kcal/kg (@ 1.790 g cm^{-3}, calcd.) [H_2O vapor][35]	4,088 [H_2O (l)][6, 17] 4,008 [H_2O (g)][17] 1,090 kcal/kg [H_2O (g)][11] 1.42 kcal/g [H_2O (l)][21] 1.36 kcal/g [H_2O (g)][21] 4,532 J/g (@ 1.655 g cm^{-3}, det. energy, cylinder test)[33] 3,596 J/g (@ 1.001 g cm^{-3}, det. energy, cylinder test)[33] 4,601 J/g (@ 1.649 g cm^{-3}, heavily confined charges) [H_2O (l)][33] 4,432 J/g (@ 1.649 g cm^{-3}, heavily confined charges) [H_2O (g)][33]

			3,676 J/g (@ 1.017 g cm^{-3}, heavily confined charges) [H_2O (l)][33] 3,550 J/g (@ 1.017 g cm^{-3}, heavily confined charges) [H_2O (g)][33] 1,090 kcal/kg (@ 1.790 g cm^{-3}) [H_2O vapor][35]
T_{ex} [K]	3,486	3,580 (@ 1.60 g cm^{-3}, calcd. BKWR)[63] 4,150 (@ 1.60 g cm^{-3}, calcd. BKWS)[63] 3,500 (@ 1.70 g cm^{-3}, calcd. BKWR)[63] 4,120 (@ 1.70 g cm^{-3}, calcd. BKWS)[63]	3,059 K (@ 1.74 g cm^{-3}) (HNS-I)[7] 3,059 K (@ 1.74 g cm^{-3}) (HNS-II)[7]
$p_{C\text{-}J}$ [kbar]	200	25.75 GPa (@ 1.82 g cm^{-3}, calcd., K-J)[28] 230 (@ 1.74 g cm^{-3}, calcd., K-J)[23] 206 (@ 1.60 g cm^{-3}, calcd. BKWR)[63] 187 (@ 1.60 g cm^{-3}, calcd. BKWS)[63] 236 (@ 1.70 g cm^{-3}, calcd. BKWR)[63] 214 (@ 1.70 g cm^{-3}, calcd. BKWS)[63]	200 (@ 1.60 g cm^{-3}) (HNS-I)[7] 241 (@ 1.74 g cm^{-3}) (HNS-I)[7] 200 (@ 1.60 g cm^{-3}) (HNS-II)[7] 215 (@ 1.65 g cm^{-3}) (HNS-II)[7] 21.5 GPa (@ 1.655 g cm^{-3})[33, 52] 7.3 GPa (@ 1.001 g cm^{-3})[33, 52]

VoD [m s^{-1}]	7,014 (@ TMD)	6,840 (@ 1.74 g cm^{-3} (TMD), R-P method)[26] 7,499 (@ TMD, calcd. CHEETAH v8.0)[27] 7,590 (@ 1.82 g cm^{-3}, calcd., K-J)[28] 7,270 (@ 1.74 g cm^{-3}, calcd., K-J)[23] 7,000 (@ 1.70 g cm^{-3})[44] 6,960 (@ 1.60 g cm^{-3}, calcd. BKWR)[63] 6,880 (@ 1.60 g cm^{-3}, calcd. BKWS)[63] 7,260 (@ 1.70 g cm^{-3}, calcd. BKWR)[63] 7,220 (@ 1.70 g cm^{-3}, calcd. BKWS)[63]	6,800 (@ 1.6 g cm^{-3})[4, 6, 7] 7,130 (@ 1.74 g cm^{-3})[5] 7,000 (@ 1.70 g cm^{-3})[29] 7,000 (@ 1.74 g cm^{-3}) (HNS-I)[7, 23] 7,410 (@ 1.74 g cm^{-3}) (HNS-I)[7] 7,000 (@ 1.70 g cm^{-3}) (HNS-I)[12, 47] 7,000 (@ 1.70 g cm^{-3}) (HNS-II)[7, 9, 12, 47] 6,800 (@ 1.60 g cm^{-3}) (HNS-I)[9] 7,200 (exptl. est., LASEM method)[27] 7,200 (@ TMD, large-scale test)[27] 7,030 (@ 1.655 g cm^{-3})[33, 52] 5,100 (@ 1.001 g cm^{-3})[33, 52] 6,800 (@ 1.60 g cm^{-3})[63] 7,000 (@ 1.70 g cm^{-3})[63]
V_0 [L kg^{-1}]	619	247.57 cm^3/mol (@ 1.82 g cm^{-3}, calcd., K-J)[28]	766[10]

Summary of experimental copper cylinder wall velocity data for homogeneous HNS, all samples have a wall thickness/diameter ratio of 0.1. All cylinders were 305 mm long. PETN with a density of 1.763 g/cm^3 is the reference explosive[51]:

Initial density (g/cm^3)	Inner diameter (mm)	Wall thickness (mm)	Wall velocity (mm/μs) @ 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
1.681	25.44	2.590	1.255	1.385	1.458	−35.3	−34.0	−33.7
1.655	25.44	2.590	1.228	1.362	1.433	−38.0	−36.2	−35.9
1.610	25.44	2.590	1.210	1.335	1.393	−39.8	−38.7	−39.4
1.597	25.44	2.590	1.229	1.340	1.413	−37.9	−38.2	−37.7
1.504	25.44	2.590	1.170	1.297	1.368	−43.8	−42.1	−41.6
1.402	25.44	2.590	1.081	1.207	1.266	−52.0	−49.9	−50.0
1.200	25.44	2.590	0.959	1.073	1.145	−62.2	−60.4	−59.1
1.001	25.44	2.590	0.817	0.931	0.981	−72.6	−70.2	−70.0

Derivation of the total energy of detonation, E_0, from the measured heat of detonation (the final state is assumed to be at 1 atm for all gaseous products, including water @ 298 K. Code calculated energies with the 1800 K freeze are also included[51]:

Measured density (g/cm^3)	Measured confined heat of detonation (kJ/cm^3)	Ref[51] densities (g/cm^3)	Heat of detonation,[51] density (kJ/cm^3)	Energy of detonation, E_0 (kJ/cm^3)			
				From heat of detonation	freeze @ 1,800 K		
					TIGER BKWR	TIGER JCZ3	CHEQ
1.649	−7.58	1.655	−7.61	−7.5	−7.3	−6.7	−7.0
1.017	−3.74	1.001	−3.68	−3.7	−3.7	−3.5	−3.8

JWL cylinder coefficients as determined in[51]:

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}
1.655	7.03	−7.50	21.5	423.7580	3.131467	1.704155	4.332	1.00	0.40	2.804
1.001	5.10	−3.60	7.3	138.8149	2.779832	0.694139	4.657	1.00	0.35	2.567

<table>
<tr><td>Critical diameter [cm]</td><td>0.5 mm (0.020 in)[21]</td></tr>
<tr><td>Critical T [°C]</td><td>320–321 (exptl.)[37, 48], 316 (calcd.)[37, 48]</td></tr>
<tr><td>Trauzl test [cm^3, % TNT]</td><td>301 cm^3[56]</td></tr>
<tr><td>USGT (underwater small scale gap test)</td><td>USGT critical length L_c = 4 mm[19]</td></tr>
<tr><td>SSGT [cm]</td><td>Critical length, L_c = 4 mm (underwater small-scale gap test)[19]

Values from[21]:

<table>
<tr><th></th><th>Density (g/cm^3)</th><th>Percent voids</th><th>Sensitivity (mm)</th></tr>
<tr><td colspan="4">NSWC SSGT</td></tr>
<tr><td>HNS-I</td><td>1.694</td><td>2.6</td><td>5.18</td></tr>
<tr><td></td><td>1.122</td><td>35.5</td><td>7.06</td></tr>
<tr><td>HNS-II</td><td>1.725</td><td>0.9</td><td>5.46</td></tr>
<tr><td></td><td>1.644</td><td>–</td><td>7.52</td></tr>
<tr><td></td><td>1.322</td><td>24</td><td>9.53</td></tr>
<tr><td colspan="4">LANL SSGT</td></tr>
<tr><td>HNS-I</td><td>1.669</td><td>4.1</td><td>5.28</td></tr>
<tr><td></td><td>1.566</td><td>10</td><td>5.84</td></tr>
<tr><td></td><td>1.376</td><td>20.9</td><td>6.71</td></tr>
<tr><td></td><td>1.840 (pressed)</td><td>2.1</td><td>2.31</td></tr>
</table>

HNS recrystallized slowly from HNS-I[55]:

<table>
<tr><th rowspan="2">Loading pressure (kpsi)</th><th colspan="2">Density (g/cm^3)</th><th>% TMD</th><th colspan="3">Sensitivity (DBG)</th></tr>
<tr><th>Avg.</th><th>s</th><th></th><th>Avg.</th><th>s_m</th><th>N</th></tr>
<tr><td>4</td><td>1.339</td><td>0.0052</td><td>77.0</td><td>4.332</td><td>0.0076</td><td>23</td></tr>
<tr><td>16</td><td>1.524</td><td>0.0049</td><td>87.6</td><td>4.833</td><td>0.0235</td><td>23</td></tr>
<tr><td>64</td><td>1.707</td><td>0.0043</td><td>95.1</td><td>6.458</td><td>0.0234</td><td>23</td></tr>
</table>
</td></tr>
</table>

HNS-1, TMD = 1.74 g cm^{-3}, (1) = no mixed response zone, (2) = test @ −65°F[55]:

Loading pressure (kpsi)	Density (g/cm^3)		% TMD	Sensitivity (DBG)			
	Avg.	*s*		Avg.	g	s_m	*N*
4	1.116	0.0136	64.1	5.507	0.0536	0.0322	20
8	1.226	0.0122	70.5	5.561	–	–	20 (1)
16	1.377	0.0067	79.1	5.779	0.0161	0.0198	20
32	1.537	0.0083	88.3	6.263	0.0240	0.0191	20
32	1.542	0.0088	88.6	6.322	–	–	20 (1)
32	1.541	0.0049	88.6	7.368	0.0167	0.0208	20 (2)
64	1.669	0.0034	95.9	6.820	0.0266	0.0224	20

HNS-I, TMD = 17.4 g cm^{-3}, (1) = no mixed response zone[55]:

Loading pressure (kpsi)	Density (g/cm^3)		% TMD	Sensitivity (DBG)			
	Avg.	*s*		Avg.	*g*	s_m	*N*
4	1.156	0.0071	66.4	5.441	–	–	20 (1)
8	1.267	0.0128	72.8	5.620	0.0069	0.0184	20
16	1.404	0.0100	80.7	5.850	0.0530	0.0315	20
32	1.529	0.0065	87.9	6.123	0.0076	0.0137	20
64	1.682	0.0026	96.7	7.173	0.0389	0.0256	20

HNS-1, TMD = 1.74 g cm^{-3}[55]:

Loading pressure (kpsi)	Density (g/cm^3)		% TMD	Sensitivity (DBG)			
	Avg.	*S*		Avg.	*g*	s_m	*N*
4	1.144	0.0109	65.7	5.843	0.0231	0.0198	20
8	1.259	0.0102	72.4	5.615	0.0140	0.0267	20
16	1.409	0.0059	81.0	5.735	0.0257	0.0174	20
32	1.555	0.0056	89.4	6.234	0.0226	0.0171	20
32	1.539	0.0045	88.4	6.058	0.0360	0.0269	18
32	1.546	0.0069	88.9	6.263	0.1345	0.0692	21
64	1.681	0.0033	96.6	7.173	0.0408	0.0267	20

Tested @ -315°F, HNS-1, TMD = 1.74 g cm^{-3}[55]:

Loading pressure (kpsi)	Density (g/cm^3)		% TMD	Sensitivity (DBG)			
	Avg.	*S*		Avg.	*g*	s_m	*N*
8	1.236	0.0136	71.0	5.724	0.1075	0.0622	19
32	1.535	0.0041	88.2	7.126	0.2234	0.1385	17

HNS-B = the sample passed the SSGT sensitivity test of WS 5003[55]:

Loading pressure (kpsi)	Density (g/cm^3)		% TMD	Sensitivity (DBG)			
	Avg.	*S*		Avg.	*g*	s_m	*N*
4	1.192	0.0134	68.5	5.058	0.0324	0.0260	20
8	1.298	0.0103	74.6	5.177	0.0727	0.0423	20
16	1.439	0.0067	82.7	5.382	0.0271	Illegible	20
28	1.527	0.0043	87.8	6.202	0.0496	0.0312	20
32	1.590	0.0084	91.4	6.399	0.0332	0.0239	20
64	1.691	0.0026	97.1	6.900	0.0536	0.0338	20

HNS-I-B = the sample passed the SSGT sensitivity test of WS 5003; (1) = no mixed response zone[55]:

Loading pressure (kpsi)	Density (g/cm^3)		% TMD	Sensitivity (DBG)			
	Avg.	*s*		Avg.	*g*	s_m	*N*
4	1.122	0.0204	64.5	5.556	–	–	18 (1)
8	1.237	0.0176	71.1	5.627	–	–	18 (1)
16	1.378	0.0184	79.2	5.856	0.0179	0.0416	18
32	1.519	0.0101	87.3	6.235	0.0292	0.0192	18
64	1.662	0.0029	95.5	7.003	0.0194	0.0167	18

HNS-I-B = the sample passed the SSGT sensitivity test of WS 5003; (1) = no mixed response zone[55]:

Loading pressure (kpsi)	Density (g/cm^3)		% TMD	Sensitivity (DBG)			
	Avg.	*s*		Avg.	*g*	s_m	*N*
8	1.351	0.0067	77.6	5.541	0.0654	0.0411	20
16	1.458	0.0044	83.8	5.856	0.0920	0.0511	20
32	1.586	0.0042	91.1	6.057	–	–	7 (1)
64	1.694	0.0060	97.4	6.903	0.0259	0.0255	18

HNS-I[55]:

Loading pressure (kpsi)	Density (g/cm^3)		% TMD	Sensitivity (DBG)			
	Avg.	*s*		Avg.	*g*	s_m	*N*
32	1.546	0.0039	88.9	6.245	0.0249	0.0190	25

HNS-II, TMD = 1.74 g cm^{-3}[55]:

Loading pressure (kpsi)	Density (g/cm^3)		% TMD	Sensitivity (DBG)			
	Avg.	*s*		Avg.	*g*	s_m	*N*
32	1.629	0.0034	93.6	5.386	–	–	10
32	1.639	0.0038	94.2	5.351	–	–	9
32	1.639	0.0034	94.2	5.295	0.0206	0.0287	10
32	1.644	0.0044	94.5	5.340	–	–	10
32	1.623	0.0035	93.3	5.412	0.0147	0.0314	10
32	1.635	0.0027	94.0	5.312	–	–	10

HNS-II, TMD = 1.74 g cm^{-3}[55]:

Loading pressure (kpsi)	Density (g/cm^3)		% TMD	Sensitivity (DBG)			
	Avg.	*s*		Avg.	*g*	s_m	*N*
32	1.624	0.0076	93.3	5.268	0.0634	0.0374	18
32	1.634	0.0060		5.366	0.0279	0.0209	20
32	1.649	0.0037	94.8	5.269	0.0546	0.0343	18
32	1.636	0.0042	94.0	5.186	–	–	19
32	1.630	0.0047	93.7	5.239	0.0251	0.0173	20
32	1.628	0.0036	93.6	5.230	0.0281	0.0195	23

HNS-II, (1) = no mixed response zone[55]:

Loading pressure (kpsi)	Density (g/cm^3)		% TMD	Sensitivity (DBG)			
	Avg.	*s*		Avg.	*g*	s_m	*N*
4	1.322	0.0107	76.0	4.264	0.0084	0.0132	18
8	1.423	0.0073	81.8	4.444	–	–	18 (1)
16	1.545	0.0044	88.8	4.767	0.0187	0.0243	18
32	1.644	0.0025	94.5	5.354	0.0168	0.0227	18
64	1.25	0.0018	99.1	6.684	0.0354	0.0274	18

<table>
<tr><td></td><td>
HNS-II, (1) = test @ −315°F[55]:
<table>
<tr><th rowspan="2">Loading pressure (kpsi)</th><th colspan="2">Density (g/cm^3)</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>32</td><td>1.627</td><td>0.0041</td><td>93.5</td><td>5.192</td><td>0.0455</td><td>0.0258</td><td>23</td></tr>
<tr><td>32</td><td>1.627</td><td>0.0040</td><td>93.5</td><td>6.757</td><td>0.1761</td><td>0.0857</td><td>23 (1)</td></tr>
</table>
Recrystallized HNS-II[55]:
<table>
<tr><th rowspan="2">Loading pressure (kpsi)</th><th colspan="2">Density (g/cm^3)</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>20</td><td>1.632</td><td>0.0020</td><td>93.8</td><td>5.306</td><td>0.0102</td><td>0.0054</td><td>20</td></tr>
<tr><td>32</td><td>1.623</td><td>0.0035</td><td>93.3</td><td>5.412</td><td>0.0147</td><td>0.0314</td><td>10</td></tr>
<tr><td>32</td><td>1.671</td><td>0.0021</td><td>96.0</td><td>5.876</td><td>0.0015</td><td>0.0010</td><td>23</td></tr>
<tr><td>32</td><td>1.628</td><td>0.0039</td><td>93.6</td><td>5.322</td><td>0.0099</td><td>0.0051</td><td>20</td></tr>
<tr><td>32</td><td>1.633</td><td>0.0021</td><td>93.9</td><td>5.539</td><td>0.0049</td><td>0.0029</td><td>20</td></tr>
<tr><td>32</td><td>1.646</td><td>0.0038</td><td>94.6</td><td>5.480</td><td>0.0350</td><td>0.0230</td><td>20</td></tr>
</table>
</td></tr>
<tr><td>Shock wave sensitivity</td><td>50% gap thickness = 8.05 mm (micro HNS)[59], 50% gap thickness = 5.10 mm (nano-HNS)[59]</td></tr>
<tr><td>5 s explosion T [°C]
Ignition T [°C]
Ignition T, 30 s delay [°C]</td><td>
354–358[44]
354 (before storage)[44], 358 (after 16 years storage in multilayered paper bags)[44]</td></tr>
<tr><td>Autoignition point [°C]</td><td>325 (HNS-I)[21], 325 (HNS-II)[21]</td></tr>
<tr><td>LLNL reactivity test</td><td>0.01 cm^3 gas evolved per 0.25 g sample @ 120 °C in 22 h[13]</td></tr>
</table>

Thermal stability

HNS-I: 0.1% dec. per h @ 260 °C[12], HNS-II: 0.1% dec. per h @ 260 °C[12]

Mass loss as function of *T* for all TGA expts., performed with constant heating rates (mass difference in %, all approx. values)[38]:

Heating rate (K/min)	*T* (°C)									
	250	270	290	300	320	340	350	370	390	400
0.05	0	0	−19	61	−67	−71	−72	−74	>−75	>−75
0.2	0	0	−5	−10	−64	−70	−72	−74	>−75	>−75
5	0	0	0	0		−32	−54	−62	−65	
10	0	0	0			−10	−29	−59	−65	
20	0	0	0			−5	−20	−52	−62	
40	0	0	0	0	0	−2	−7	−34	−62	−65

Mass loss as function of time for TGA expts., performed with constant *T* (mass difference in %, all approx. values)[38]:

T (°C)	Time (min)					
	0	120	240	360	480	600
254	0	−1	−1	−1	−1	−2
274	0	−3	−4	−7	−10	−12
289	0	−5	−13	−25	−34	−57
304	0	−37	−64	−66	−67	−68

Stable @ 260 °C but dec. @ higher T[49], 0.1%/h dec. rate @ 260 °C (HNS-I)[21], 0.1%/h dec. rate @ 260 °C (HNS-II)[21], 0.50 cc/g/h @ 260 °C for 2 h[57]

No significant weight loss occurs using accelerated aging measurements in vacuum @ 84 °C (Quartz spring balance apparatus) over 297 days for HNS-IIA (equivalent to 9.9 years @ 66 °C)[62], no significant changes in DTA of HNS-IIA after 183 of accelerated aging (equivalent to 6.1 years)[62], no significant changes in DTA of HNS-IIA which had undergone two rounds of sterilization cycles (125 °C for 64 h each) prior to 94 days of accelerated aging equivalent to 3.1 years[62]

Vacuum stability test [cm^3/h]

@ 200 °C total vol. of gas (cm^3) evolved/no. of days[25]: 0.4/2, 0.7/7, 1.0/14, 1.2/21, 1.4/28, 1.6/35, 1.7/42, 1.8/49, 2.0/56, 2.3/63, 2.5/70, 2.6/77, 2.8/84, 3.0/91[25]

@ 175 °C total vol. of gas (cm^3) evolved/no. of days[25]: 0.2/2, 0.4/7, 0.5/14, 0.6/21, 0.7/28, 0.8/35, 0.8/42, 0.9/49, 1.0/56, 1.1/63, 1.1/70, 1.2/77, 1.2/84, 1.2/91[25]

	HNS-I[12, 21]	HNS-II[12, 21]
@ 260 °C: First 20 min (cc/g/h)	1.8	0.3
@ 260 °C: Additional 2 h (cc/g/h)	0.6	0.2
@ 280 °C	2.7	2.7

1.68 cc/g/h @ 260 °C (grade I)[58], 0.50 cc/g/h @ 260 °C (recryst. from nitrobenzene)[58], 0.23 cc/g/h @ 260 °C (grade II)[58], 0.5 cc/g/h, 82 h period) @ 260 °C[61]

Vapor pressure [atm. @ °C]

1×10^{-9} mm Hg @ 100 °C (HNS-II)[13], 2.88×10^{-14} Torr @ 66 °C[18], 1.33×10^{-7} Pa @ 20 °C[47], HNS-I: 2.9×10^{-8} mm Hg @ 160 °C[12, 21], HNS-II: 2.9×10^{-8} mm Hg @ 160 °C[12, 21], 0.396×10^{-7} Torr @ 161.4 °C[47], 0.592×10^{-7} Torr @ 166.4 °C[47], 2.15×10^{-7} Torr @ 177.3 °C[47], 4.97×10^{-7} Torr @ 185.8 °C[47], 39.4×10^{-7} Torr @ 206.3 °C[47]

Values from[50]:

T (°C)	Vapor pressure (x 10^7 Torr)	wt. loss (g × 10^3)	Time (sec)
161.4	0.396	4.10	688,680
166.4	0.592	12.8	578,880
177.3	2.15	22.9	288,000
185.8	4.97	12.25	168,480
206.3	39.4	36.55	64,800

Sublimation rates used to calculate the vapor pressure (HNS-IIA)[62]:

T (°C)	wt. loss rate (mg/h)	Sublimation (g/cm^2/sec)	Vapor pressure (Torr)
132	6.24×10^{-4}	2.63×10^{-10}	4.28×10^{-9}
139	2.75×10^{-2}	1.02×10^{-8}	1.67×10^{-7}
150	3.75×10^{-2}	1.42×10^{-8}	2.34×10^{-7}

Solubility [g/mL]

Fairly insoluble in most common organic solvents[39], soluble in DMF, NMP (*N*-Methylpyrrolidinone), CH_3CN, THF[39], 0.22 mg/L in H_2O @ 20/25 °C[47]

Solubility g/100 mL solvent @ 25 °C[47]: 1.940 in NMP, 1.310 in DMF, 1.210 in DMSO, 0.569 in NMP & 5% H_2O, 0.541 in 4-Butyrolactone, 0.475 in propylene carbonate, 0.452 in 25% ACN & 75% DMF, 0.261 in NMP & 2.5% H_2O, 0.195 in acetophenone, 0.175 in 50% ACN & 50% DMF, 0.124 in cyclohexanone, 0.069 in 75% ACN % 25% DMF, 0.064 in 1,2-dimethoxyethane, 0.062 in ACN, 0.056 in bis(2-methoxyethyl) ether, 0.047 in p-dioxane, 0.044 in methyl ethyl ketone, 0.037 in ethyl acetate, 0.030 methyl formate, 0.024 ethyl formate, 0.017 *n*-propyl formate, 0.014 in 2-methoxyethanol, 0.011 in ethoxybenzene, 0.007 in 1,2-dichloroethane, 0.006 in dichloromethane, 0.006 in ethyl lactate, 0.04 in 3-methylphenol, 0.003 in 2-chloroethanol, 0.002 in chlorobenzene, 0.02 in 2-ethoxy ethanol, 0.002 in propanol, 0.001 in $CHCl_3$, 0.001 in cylcohexanol, 0.000 in EtOH, 0.000 in MeOH[47]

Solubility @ 30 °C, 40 °C and 60 °C in g/100 mL solvent[47]:

Solvent	$T = 30$ °C	$T = 40$ °C	$T = 60$ °C
Nitrobenzene	0.059	0.072	0.094
Methyl ethyl ketone	0.035	0.052	0.061
Acetone	0.064	0.075	0.131
MeOH	0.003	0.006	0.008
DMF	1.312	1.703	2.198
CH_3CN	0.043	0.064	0.084
Cyclohexanone	0.118	0.156	0.206

Soluble in hot nitrobenzene and DMF[49], slightly soluble in hot glacial acetic acid, acetone or methyl ethyl ketone[49], soluble in DMF[21], slightly soluble in hot acetone, methyl ethyl ketone and glacial acetic acid[21]

Solubility of HNS (g/10 g solvent) after 5 min stirring (* @ bpt. of solvent)[53]:

Solvent	25 °C	60 °C	80 °C	98 °C
DMSO	1.4	2.4	3.6	9.1
DMF	1.5	3.2	4.6	7.0
N-Methylpyrrolidinone	2.4	4.6	6.4	8.4
Butyrolactone	0.4			3.2
Dimethylacetamide	1.2			5.4
Acetone	< 0.1	0.4*		
Nitrobenzene	< 0.1			0.8
Hexamethylphosphoramide				3.3
Cyclohexanone				1.1

Soubility in binary solvent mixtures @ 25 °C (g HNS/100 g solvent) after 5 min stirring[53]:

Solvent	Solubility (g HNS/100 g solvent)
DMSO	1.4
NMP	2.4
NMP 79.2% DMSO 20.8%	2.3
DMF	1.5
DMF 71.7% DMSO 28.3%	1.7
Butyrolactone	0.4

Comparison of solubilties (g/100 g solvent) in DMSO after 5 and 30 min stirring @ 25 °C[53]: 1.4 g HNS after 5 min[53], 1.4 g HNS after 30 min[53]

Recryst. from nitrobenzene[57], slightly soluble in acetone and boiling acetone[57], soluble in hot nitrobenzene, DMF, almost insoluble in cold nitrobenzene or DMF[57], slightly soluble in hot glacial acetic acid, acetone or methyl ethyl ketone[57], insoluble in MeOH and hexane[57], recryst. from DMF[57], extremely low solubility in most common organic solvents[58]

<table>
<tr><td>Surface area</td><td>Typical surface area resulting from crash precipitation into H_2O of HNS solns. with various solvents[39]:

<table><tr><th>Crash precipitation solvent</th><th>Specific surface area (m^2/g)</th><th>Solvent content (wt.%)</th></tr><tr><td>DMF</td><td>9–19</td><td>0.2–1.2</td></tr><tr><td>NMP†</td><td>16–21</td><td>0.6–0.9</td></tr><tr><td>CH_3CN</td><td>6–12</td><td>0.1</td></tr><tr><td>THF</td><td>16–20</td><td>0.2–0.3</td></tr></table>
† = N-Methylpyrrolidinone</td></tr>
<tr><td>Short duration shock wave sensitivity [mJ]</td><td>249 (ultra-fine HNS by spray drying, electrically exploded metal-foil-driven flyer)[40], 960 (synthesized HNS, electrically exploded metal-foil-driven flyer)[40]</td></tr>
<tr><td>Cook-off (T_c) [°C]</td><td>312 (heating rate @ 1 °C/min until cook-off registered as temperature jump, prior to cook-off no melting observed, curve has no plateau before the T jump)[44]</td></tr>
<tr><td>K_{ow}</td><td>112[47]</td></tr>
<tr><td>K_{oc}</td><td>86[47]</td></tr>
<tr><td>Enthalpy of sublimation [kcal/mol]</td><td>94.9 cal/g (heat of subl.)[21], 43.01[47], 43.01 kcal (molar heat of sublimation)[50], 95.5 cal/g (specific heat of sublimation)[50]</td></tr>
<tr><td>Sublimation rate</td><td>Sublimation rates @ 82–150 °C for 216 h test period showed no measurable weight loss at lower T (HNS-IIA)[62]. At $T \geq 132$ °C[62]:

<table><tr><th>T (°C)</th><th>wt. loss rate (mg/h)</th><th>Sublimation (g/cm^2/s)</th><th>Vapor pressure (Torr)</th></tr><tr><td>132</td><td>6.24×10^{-4}</td><td>$2.63 \times 10^{-1}0$</td><td>4.28×10^{-9}</td></tr><tr><td>139</td><td>2.75×10^{-2}</td><td>1.02×10^{-8}</td><td>1.67×10^{-7}</td></tr><tr><td>150</td><td>3.75×10^{-2}</td><td>1.42×10^{-8}</td><td>2.34×10^{-7}</td></tr></table></td></tr>
<tr><td>Enthalpy of vaporization [kcal/mol]</td><td>19.9 (calcd.)[47]</td></tr>
<tr><td>Diffusion [m^2/s]</td><td>4.5×10^{-6} @ 20 °C (in air)[47], 3.9×10^{-9} @ 20 °C (in water)[47]</td></tr>
<tr><td>Particle size</td><td>1–5 microns (HNS-I)[21], 100–300 microns (HNS-II)[21]</td></tr>
<tr><td>Bridge wire</td><td>Mean firing voltage for explosive bridge wire with 1 mF capacitor: 12.950 V (@ 0.9 g cm^{-3}, HNS-I)[21], 12,950 V (@ 0.9 g cm^{-3}, HNS-II)[21]</td></tr>
</table>

<table>
<tr><td>Laser ignition</td><td>Ignition power threshold, ignition and full burn delay times (@ 45 W) for HNS IV and its mixtures with the dye and CB (continuous wave diode laser, CB = carbon black powder, dye with molecular formula $C_{54}H_{54}N_2O_4S$ with an absorption band at 811 ± 25 nm, HNS V mean particle size = 44 µm)[54]:
<table>
<tr><td>Sample for ignition</td><td>HNS IV/dye</td><td>HNS IV/CB</td><td>Pure HNS IV</td></tr>
<tr><td>Threshold power [W] ± 0.2</td><td>4</td><td>4</td><td>Not ignited up to 45 W</td></tr>
<tr><td>Ignition delay [ms] ± 10% (@ 45 W)</td><td>2.1</td><td>1.2</td><td>-</td></tr>
<tr><td>Full burn time [ms] ± 10% (@ 45 W)</td><td>2.6</td><td>2.8</td><td>-</td></tr>
</table></td></tr>
<tr><td>Fragment sensitivity</td><td>Summary of fragment sensitivity, chemical assay and surface area analysis for HNS[60]:
<table>
<tr><td rowspan="2">HNS type</td><td rowspan="2">Approx. 50% fire acceptor closure thickness (in)</td><td colspan="3">HPLC assay</td><td rowspan="2">Surface area analysis (cm^2/cm^3)</td></tr>
<tr><td>% HNS</td><td>% HNBiB</td><td>% TNB</td></tr>
<tr><td>I</td><td>0.020</td><td>99.5</td><td>0.5</td><td>None</td><td>128,336</td></tr>
<tr><td>I</td><td>0.020</td><td>93.0</td><td>6.7</td><td>None</td><td>67,297</td></tr>
<tr><td>I</td><td>0.020</td><td>97.8</td><td>1.9</td><td>0.3</td><td>52,165</td></tr>
<tr><td>I</td><td>0.020</td><td>94.5</td><td>4.6</td><td>0.1</td><td>47,929</td></tr>
<tr><td>I</td><td>0.017</td><td>99.2</td><td>0.6</td><td>Trace</td><td>26,818</td></tr>
<tr><td>II</td><td>0.010</td><td>99.5</td><td>0.2</td><td>None</td><td>8,996</td></tr>
<tr><td>II</td><td>0.010</td><td>99.6</td><td>None</td><td>None</td><td>8,996</td></tr>
<tr><td>II</td><td>0.010</td><td>98.7</td><td>None</td><td>None</td><td>7,612</td></tr>
</table></td></tr>
</table>

	HNS[13, 14, 57]	**HNS[15]**	**HNS[16, 47]**	**HNS-I[17]**
Chemical formula	$C_{14}H_6N_6O_{12}$	$C_{14}H_6N_6O_{12}$	$C_{14}H_6N_6O_{12}$	$C_{14}H_6N_6O_{12}$
Molecular weight [g mol^{-1}]	450.23	450.23	450.23	450.23
Crystal system	Orthorhombic	Monoclinic	Monoclinic	Orthorhombic
Space group		$P\,2_1/\,c$ (no. 14)	$P\,2_1/\,c$ (no. 14)	

a [Å]	20.93	22.326(7)	22.083(6)	22.13
b [Å]	5.57	5.5706(9)	5.554(1)	5.57
c [Å]	14.67	14.667(2)	14.634(3)	14.67
α [°]	90	90	90	90
β [°]	90	110.04(1)	108.45(2)	90
γ [°]	90	90	90	90
V [Å^3]		1,713.68	1,702.59	
Z		4	4	
ρ_{calc} [g cm^{-3}]		1.745, $D_m = 1.74(1)$	1.756	
T [K]		295	295	

Crystal expansion of HNS at different temperatures, X-ray powder diffraction[47]:

T (°C)	a (Å)	b (Å)	c (Å)	β (°)	V (Å^3)	ρ (g cm^{-3})
30	22.3472	5.5753	14.6698	110.05	1,716.98	1.7418
60	22.3927	5.5851	14.6740	110.00	1,724.51	1.7342
90	22.4400	5.5961	14.6798	109.96	1,732.67	1.7260
120	22.4915	5.6076	14.6864	109.92	1,741.49	1.7172
150	22.5382	5.6174	14.6889	109.88	1,748.94	1.7099
180	22.5931	5.6300	14.6947	109.83	1,758.29	1.7008
210	22.6501	5.6431	14.7015	109.79	1,768.10	1.6914
240	22.7062	5.6542	14.7025	109.74	1,776.61	1.6833
210	22.6465	5.6422	14.6987	109.79	1,767.19	1.6923
180	22.5928	5.6308	14.6954	109.83	1,758.58	1.7006
150	22.5403	5.6190	14.6891	109.87	1,749.63	1.7093
120	22.4833	5.6059	14.6796	109.91	1,739.58	1.7191
90	22.4370	5.5960	14.6740	109.95	1,731.85	1.7268
60	22.3901	5.5855	14.6684	110.00	1,723.83	1.7348
30	22.3450	5.5757	14.6640	110.043	1,716.34	1.7424

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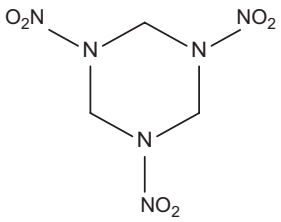
Hexogen

Name [German, acronym]: 1,3,5-Trinitro-1,3,5-triazacyclohexane, 1,3,5-trinitro-1,3,5-triazinane, cyclotrimethylenetrinitramine, hexahydro-1,3,5-trinitro-1,3,5-triazine, cyclonite, royal demolition explosive [hexogen, RDX, E-Salz, K-Salz, KA-Salz, SH-Salz, W-Salz, T4, CTMTN][†]

Main (potential) use: Secondary (high) explosive, presently used in munitions fillers such as composition A, composition B, composition C and cyclotols[156], ingredient in plastic explosives[156], explosive "fill" in most types of munitions compounds[156], component of bursting charges for aerial bombs, mines and torpedoes[156], used alone as base charge in detonators[159], if desensitized as subbooster, booster or bursting charge[159], mainly used in mixtures (compositions A, B, B-2, C, C-2, C-3 and C-4), Torpex, PTX-1 and PTX-2[169], can be used on its own as booster, subbooster and bursting charge[169], extensively as base charge in detonators[20], ingredient in castable TNT-based binary explosives for example, composition B[20], primary ingredient in plastic bonded explosives for example, composition A or composition C[20]

Structural formula:



[†] Type A and type B RDX are made by different manufacturing processes, type A contains no HMX whereas type B contains 8–12% HMX impurities[19], RDX type A is made by the nitric acid process, type B is made by the acetic anhydride process[43], RS-RDX refers to reduced-sensitivity RDX[111]; RDX-Type I is prepared by the Woolwich process[111]; type A must have minimum mpt. of 200 °C and max. acidity of 0.05% (as nitric acid)[169], type B must have minimum mpt. of 190 °C and max acidity of 0.02% (as acetic acid)[169]; type B is less pure than type A (HMX is main impurity)[169]

	RDX
Formula	$C_3H_6N_6O_6$
Molecular mass [g mol^{-1}]	222.12

Appearance at RT	White crystals[80], recryst. from nitrobenzene as needles[80], recryst. from hot acetone as sparkling prisms[80], white crystalline solid[153, 156], colorless, orthorhombic crystals[159], colorless or white solid[169], white, odorless and tasteless crystals[172], colorless polycrystalline solid[20]
IS [J][16]	7.5 (<100 µm), 5.90[1], 7.4 Nm[2], 7.5[4, 112], 6.69 (1st reaction)[7, 96], 5.90 (sound)[7, 96], 5.58[9, 10], 300% as sensitive as TNT[19], 7 (BAM, 2 kg)[39], H_{50} = 24 cm[10], 34[27], $H_{50\%}$ = 24 cm (US-NOL apparatus)[30], $H_{50\%}$ = 24 cm (2.5 kg hammer, 35 mg sample, US Naval lab)[84], H_{50} = 22 cm (tool type 12)[20], H_{50} = 41 cm (tool type 12B)[20], H_{50} = 28 cm (tool type 12, 5 kg mass)[24], $H_{50\%}$ = 24 cm (LASL test)[25], 8–9 in (18 mg sample, 2 kg mass, P.A.)[29], 34–40 cm (RDX type B, 2 kg mass, B.M.)[29], 42 cm (2 kg mass, European impact machines)[29], drop energy required for 50% initiation probability = 6.69 (25 mg sample, Julius-Peters apparatus)[36], drop weight = 3.5–7.5 Nm[37], 25 cm (B.M., tool type 12, 2 kg)[41], $Ed_{min.}$ = 25 (BAM, 5 kg mass, max. level with six consecutive negative runs)[43], Rotter FOI = 80[44], 30–35 cm (US drophammer)[44], 28 cm (ERL type 12)[50], 23–28 cm (ERL-LASL type 12)[26], 32–42 cm (B.M., 2 kg mass)[26], 30 cm (ERL)[67], 3.5 (BAM, Julius-Peters)[68], H_{50} = 26 cm[73], >3.52 (micron-sized RDX)[76], >3.52 (nanosized RDX)[76], 29.8 cm (7.3 J)[77], 22 cm (NEDED)[78], 24 cm (NOL)[78], 28 cm (LANL)[78], exploded by 9 in (2 kg mass)[80], $H_{50\%}$ = 22 in (10 µm, Thiokol app.)[81], 3.5 cm (10 µm, ABL app.)[81], $(H_{50}Wg)^{-1}$ = 7.4 Nm[86], $H_{50\%}$ = 16–33 cm[89], $H_{50\%}$ = 25–30 cm (500 g hammer)[84], 24 cm (Bruceton method, type 12 tool, 2.5 kg mass, 40 mg sample, 5/0 sandpaper, 25 trials)[98], 38 cm (2 kg mass, BAM)[103], H_{50} = 42 cm (2 kg hammer, E_{d50} = 8.4 J)[113], 5 (ground RDX)[117], 5 Nm[121], 4.0 Nm (ball milled)[121], 7.5 Nm (RDX processed by PCA method (precipitation by the compressed fluid antisolvent))[121], H_{50} = 24.2 cm (Bruceton method, NOL machine, type 12 tool, 2.5 kg mass, 35 ± 2 mg sample, 5/0 sandpaper)[127], >1.56 (nanostructured RDX)[128], >3.52 (nanostructured RDX/wax composite)[128], 80% explosion probability (@ 25 cm drop height, 10 kg mass, 50 mg powder sample between two hardened anvils, 25 tests, WL-1 apparatus)[132], 7.1 (2 kg mass, Julius-Peters)[134], 7.4[134], 8.5[136], Ed_{min} = 25 (BAM, 5 kg mass, RT)[138], 5.0 Nm (raw RDX, $X_{50.3}$ = 21.7 µm, 1.902 g cm^{-3})[142], 4.0 Nm (milled RDX using annular gap ball mill, $X_{50.3}$ = 0.66 µm, 1.942 g cm^{-3})[142], 7.5 Nm (RDX micronization by PCA process, $X_{50.3}$ = 10.8 µm, 1.811 g cm^{-3})[142], H_{50} = 26 cm (2.5 kg mass, type 12 tool)[148], 1279 mm (dropheight, Rotter impact test)[151], 1386 mm (dropheight, Rotter impact test, +5% DETA)[151], 25–35 cm (0.5 kg mass)[157], 32 cm (2 kg mass, 20 mg sample, B.M.)[164], 8 in (2 kg mass, 18 mg sample, P.A.)[164], 16 in (2 kg mass, confined, height of no detonation, P.A.)[165], 32 cm (2 kg mass, B.M.)[169], 8 in (2 kg mass, P.A.)[169], 80% sensitivity @ 25 cm (10 kg mass)[172], 30–32 cm (2 kg mass)[172], 8 in (18 mg sample, P.A.)[174], 32 cm (B.M.)[174], 8 in (18 mg sample, P.A.)[174], 100+ cm (B.M)[174], 24 cm (average, 50% point, type 12 tool, 2.5 kg mass, sandpaper)[179], 5.8 (micro-RDX)[187], 13.5 (nano-RDX, milling method)[187], 18.8 (nano-RDX, RESS method)[187], >3.52 (raw material, microsized)[189], >3.52 (nanostructured)[189], 7.5 (conventional RDX)[189], 10 (submicrometer, 499 nm diameter, cryst. using electrospray technique)[189], 5 (conventional RDX)[189], 5 (submicrometer RDX, 500 nm diameter, plasma method)[189], A_{d1} = 80%, A_{d2} = 92%, LL = 0.7 m, $A_{50\,d1}$ = 1.7 m, $A_{50\,d2}$ = 0.8[22], 7.5[194]

Rotter FoI = 80[26], gas evolution = 18 mL[26], average powder explosiveness = 51[26]

IS at various temperatures using P.A. apparatus (2 kg mass)[19, 164]: 9 in @ RT[19, 164], 8 in @ 32.2 °C[19, 164], 5 in @ 104 °C[19, 164]
IS at various temperatures using P.A. apparatus[19]: 9 in @ 20 °C[19], 8 in @ 88 °C[19], 5 in @ 105 °C[19]

RDX (standard): median height = 104 cm (5 kg mass, 30 mg sample, Rotter apparatus)[33]
RDX (military grade): median height = 98 cm (5 kg mass, 30 mg sample, Rotter apparatus)[33]

Powdered samples: $H_{50\%}$ = 24 cm (NOL), $H_{50\%}$ = 22 cm (LASL), $H_{50\%}$ = 79 cm (B.M. ERL), $H_{10\%}$ = 32 cm (P.A., BM), $H_{10\%}$ = 8 in (P.A.)

Aging samples (aging was performed as isothermal @ 70 °C for 113 days in absence of air and moisture)[23]: fresh RDX E_{50} = 8.0 (BAM)[23], aged RDX E_{50} = 8.3[23]

7 (H_{50} = 14 cm, phlegmatized RDX, 5 kg hammer, H_{50} = highest drop height at which no reaction was observed)[64]

Size, density and sensitivity of RDX crystalline particles (C-RDX = commonly used RDX, D-RDX = desensitized RDX)[65]:

Material	Mean size d_{50} (µm)	Average crystal ρ @ 20 °C (g cm^{-3})	Exploding probability hammer: 10 kg sample: 50 mg drop height: 25 cm
C-RDX	186	1.7913 ± 0.0005	80% $(0.61, 0.90)_{0.95}$
D-RDX	283	1.7992 ± 0.0003	70% $(0.50, 0.87)_{0.95}$

Drop height = 1.05 m, sample thickness = 1.0–2.0 mm, drop weight = Al alloy plate with mass ~5.5 kg, impact velocity from max. drop height = ~4.5 ms^{-1} producing a max. impact pressure of ~1 GPa[83]:

Material	Pellet diameter (mm)	ρ (% TMD)	No. of tests	% positive
Conventional RDX (powders with grain sizes of 10–200 μm)	4	90	3	0
	8	83	3	0
	4	46–49	3	0
	6	50–57	5	60
Ultrafine RDX (powders with micron-sized grain sizes)	8	44–51	3	0
	4	87–92	3	0
	8	75–80	3	0

Drop height = 1.3 m, sample thickness = 1.0–2.0 mm, drop weight = Al alloy plate with mass ~5.5 kg [83]:

Material	Pellet diameter (mm)	ρ (% TMD)	No. of tests	% positive
Conventional RDX (powders with grain sizes of 10–200 μm)	4	78–94	22	9
	6	77–90	3	0
	8	79–82	3	0
	4	38–65	10	60
	6	40–59	5	40
Ultrafine RDX (powders with micron-sized grain sizes)	8	42–49	3	0
	4	72–92	21	10
	6	83–85	3	0
	8	74–78	3	0

Particle size data and IS for RDX powders[126]:

RDX sample	Particle size data (µm)		IS†	
	Median	16–84% prob. range	Rotter FoI	Gas evolved (mL)
Grade A, 250–300 µm sieve cut	250	220–30	75	14.5
Grade A, 125–150 µm sieve cut	138	95–179		
Grade A, 75–106 µm sieve cut	100.0	73.3–138.0		
Grade E	21.5	10.8–36.0		
Ball-milled	3.9	~ 1–9.4	85	17

RDX grade A = Albion Explosives Factory, H_2O wet supplied, dried before use; RDX grade E = Weapons Systems Research Laboratory (WSRL), H_2O wet supplied, dried before use, RDX ball-milled = nominal size 4, supplied H_2O wet by WSRL, ball-milling carried out on grade A RDX under inert solvent; † Rotter apparatus, 5 kg mass, Bruceton method, (values rel. to RDX grade G = 80), height for 50% initiation probability[126]

Comparison of IS data of ERL and B.M.[130]:

RDX sample type manufacturer	NSWC data, H_{50} (cm)	NAVAIR data H_{50} (cm)	AFRL data H_{50} (cm)
ADI (Australia)	20	20	19
BAE HSAAP OSI (USA)	22	19	23
BAE-RO (UK)	21	23	19
Dyno Type II (Norway)	21	20	18
Dyno RS-RDX (Norway)	16	21	17.5
I-RDX	19	20	17
MI-RDX	24	17	22

IS for different RDX samples[143]:

RDX type	Manufacturer	$X_{50.3}$ (µm)	IS (Nm)
Type 1, class 1	Dyno Nobel ASA	194.5	7.5
Type 1, class 5	Dyno Nobel ASA	17.6	10
RS-RDX type 1 class 1	Dyno Nobel ASA	205.2	7.5
RS-RX, type 1, class 5	Dyno Nobel ASA	9.7	10
Hexogen, i-RDX, class 1	Eurenco, Groupe SNPE	225.4	7.5
Hexogen, i-RDX M3C	Eurenco, Groupe SNPE	10.5	7.5

RDX/wax (ERL apparatus, No. 12): 34 (99/1), 35 (98/2), 43 (97/3), 47 (95/5)[174]
RDX/calcium stearate (ERL apparatus, No. 12): 23 (98.6/1.4), 37 (98.0/2.0), 32 (97.2/2.8)[174]

IS as a function of RDX type and particle diameter, H_{50} (cm), approx. values[189]:

	Particle diameter		
	200 nm	500 nm	4 µm
Wax-coated RDX	47	63	27
Uncoated RDX	58	73	33

IS with Rotter apparatus, 5 kg mass, cf. FoI for RDX = 80 as standard[198]:

Explosive	Median height	FoI
RDX military grade	98	75
RDX standard	104	80
RDX/wax, 91/9	127	98
RDX/TNT, 60/40	137	105
RDX/TNT/wax	152	117
RDX/TNT/Al/wax	190	146

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[200]:

Rotter impact data		US data	
F of I	gas evolved (mL)	NSWC/NOL, ERL type 12	NWC B.M. type 12
80	17.9	24	19

Rotter impact data, 20 drop expts., $H_{50\%}$ = median drop height, each drop expt. has the no. of ignitions out of 20 (n_g), the fraction of ignitions (P_g), average gas volume evolved per ignition (V_g) and calcd. powder explosiveness at each level (X), RDX grade A, $H_{50\%}$ = 105 cm, data from[200]:

Drop height multiple of $H_{50\%}$	No. of fires out of 20 drops (n_g)	$P_g = n_g/20$	Average gas evolved, V_g (ml)	Explosiveness at each level, × (%)
0.67	1	0.05	17.0	62.3
0.75	1	0.05	18.0	63.3
1.0	10	0.5	14.0	50.4
1.5	20	1.0	13.1	47.8
2.0	10/10	1.0	13.7	53.9

FS [N]

120 (<100 µm), 120[2, 4, 112], 148.5[8–10], 20 (P.A.)[15, 16], 13.73 (E.R.L.)[15, 16], $P_{fr.LL}$ = 270 MPa[22], $P_{fr.50\%}$ = 480 MPa[22], 120 (up–down method)[39], 407 lbs (ABL pendulum friction test)[41], $G_{min.}$ = 160 N (BAM, Julius-Peters, max. level with six consecutive negative runs)[43], Rotter mean figure of friction (FOF) = 3.0[35], BAM (mean limiting load) = 173[35], >360 (BAM)[26], 193 (BAM, Julius-Peters)[68], 250 Nm (50% value, BAM)[69], 160 (micron-sized RDX)[76], >360 (nanosized RDX)[76], 168[77], 130 psi @ 4 ft/s (10 µ)[81], Rotary FoF = 3.0[94], Rotary FoF = 3.4[94], 173 (BAM, limiting load)[94], 120 (BAM, limiting load)[94], torpedo friction = 10–20 cm (1 kg @ 80 °C, 0.5 m/s)[84, 157], 120 (Julius-Petri)[103], 120 (ground RDX)[117], 120[121], 96 (ball milled)[121], 96 (RDX processed by PCA method (precipitation by the compressed fluid antisolvent))[121], >360 (nanostructured RDX)[128], >360 (nanostructured RDX/wax composite)[128], 76% explosion probability (powder sample between one fixed and one movable stainless steel plate, 25 tests, WM-1 apparatus)[132], H_{50} = 29.4 cm (σ = 0.326 cm, raw RDX crystal, mean particle size = 127 µm, 5 kg hammer, Bruceton method)[133], H_{50} = 44.5 cm (σ = 0.205 cm, granular-shaped RDX, mean particle size = 2.5 µm, 5 kg hammer, Bruceton method)[133], H_{50} = 34.9 cm (σ = 0.537 cm, irregular-shaped RDX, mean particle size = 4.5 µm, 5 kg hammer, Bruceton method)[133], 191[136], G_{min} = 160 (BAM Julius Peters, max level with 6 consec. negative runs)[138],

120 (raw RDX, $X_{50.3}$ = 21.7 µm, 1.902 g cm^{-3})[142], 96 (milled RDX using annular gap ball mill, $X_{50.3}$ = 0.66 µm, 1.942 g cm^{-3})[142], 96 (RDX micronization by PCA process, $X_{50.3}$ = 10.8 µm, 1.811 g cm^{-3})[142], explodes with steel shoe (friction pendulum test)[19, 164], unaffected by fiber shoe (friction pendulum test)[19, 164], no detonation with fiber shoe, detonates if struck with steel shoe (B.M.)[80], partial deflagration occurs if rubbed in unglazed porcelain mortar[19], explodes with steel shoe in Picatinny friction test[174], 216 (micro-RDX)[187], 216 (nano-RDX, milling method)[187], 216 (nano-RDX, RESS method)[187], 160 (raw material, microsized)[189], >360 (nanostructured)[189], 120 (conventional RDX)[189], >360 (submicrometer, 499 nm diameter, cryst. using electrospray technique)[189], 144 (conventional RDX)[189], >360 (submicrometer RDX, 500 nm diameter, plasma method)[189], 120[194]

Mallet FS[35]: steel on steel = 50%[35], nylon on steel = 0%[35], wood on softwood = 0%[35, 181], wood on hardwood = 0%[35, 181], wood on Yorkstone = 0%[35, 181]

Influence of humidity on FS[41]:

T / °C	Rel. humidity (%)	Abs. humidity (kPa)	Load for 50% ignitions (kg)
22	84	2.22	5
22	50	1.32	2
22	20	0.53	0.5
30	50	2.12	2
30	20	0.85	0.5
40	28	2.07	1

Aging samples (aging was performed as isothermal @ 70 °C for 113 days in absence of air and moisture)[23]: fresh RDX F_{50} = 182 (BAM)[23], aged RDX F_{50} = 172[23]

FS for different RDX samples[143]:

RDX type	Manufacturer	$X_{50.3}$ (µm)	FS (N)
Type 1, class 1	Dyno Nobel ASA	194.5	160
Type 1, class 5	Dyno Nobel ASA	17.6	168
RS-RDX type 1 class 1	Dyno Nobel ASA	205.2	160
RS-RX, type 1, class 5	Dyno Nobel ASA	9.7	144
Hexogen, i-RDX, class 1	Eurenco, Groupe SNPE	225.4	96
Hexogen, i-RDX M3C	Eurenco, Groupe SNPE	10.5	112

<table>
<tr>
<td>ESD [J]</td>
<td>0.15–0.20, 2.49[1, 3], 216.4 mJ[3], 0.2[4], >0.25 (ERL apparatus)[41], spark sensitivity: 0.2 (3 mil foil)[50], 0.037[67], 180–≥726 mJ[68], 119.42 mJ (micron-sized RDX)[76], 268.69 mJ (nanosized RDX)[76], $E_{50\%}$ = <0.03 (10 µ)[81], >156 mJ (closed container)[123], >156 mJ (open container)[123], 215.34 mJ (nanostructured RDX)[128], 374.09 mJ (nanostructured RDX/wax composite)[128], E_{50} = 1.11 (average diameter in cubage of RDX = 132.65 µm, rel. surface area = 803 $m^2 kg^{-1}$, discharging distance = 0.5 mm, GJ B736 11–90 standard method, capability of capacitance = 0.212 µF, @ 20 °C, rel. humidity = 48%)[131], $E_{0.01}$ = 0.37 (average diameter in cubage of RDX = 132.65 µm, rel. surface area = 803 $m^2 kg^{-1}$, discharging distance = 0.5 mm, GJ B736 11–90 standard method, capability of capacitance = 0.212 µF, @ 20 °C, rel. humidity = 48%)[131], E_{50} = 0.3551 (V_{50} = 4.824 kV, JGY-50 apparatus)[132], 0.32–1.8 mJ (old equipment, different particle sizes), >5,600 mJ (medium particle size of 192 µm, new equipment)[141], 0.25 (micro RDX)[187], 0.25 (nano-RDX, milling method)[187], 0.25 (nano RDX, RESS method)[187], 120 mJ (raw material, micro sized)[189], 270 mJ (nanostructured)[189], >250 mJ[194]

Spark sensitivity: 0.22 (brass electrode, 3 mils Pb foil thickness)[20], 0.55 (brass electrode, 10 mils Pb foil thickness)[20], 0.12 (steel, 1 mil Pb foil thickness)[20], 0.87 (steel, 10 mils Pb foil thickness)[20]

Min. equivalent voltages @ 0.0003 mfd; local ignition 14,950 (RDX pulverized or crystalline), no ignition @ 12,300 (RDX pulverized or crystalline)[29]

Aging samples (aging was performed as isothermal @ 70 °C for 113 days in absence of air and moisture): fresh RDX E_{50} = 55 mJ[23], aged RDX E_{50} = 67 mJ[23]

$E_{50\%}$ = 0.15 ± 0.03 (Bruceton formula)[85], $E_{50\%}$ = 0.12 ± 0.03 (Bruceton formula)[85], $E_{50\%}$ = 0.21 (LANL using 0.008 cm Pb foil confinement)[85]

No ignitions @ 12,300 V, but local ignitions @ 14,950 V (circuit with capacitance of 0.0003 mF, pulverized or crystalline sample)[19]

0.100 (20,000 voltage, for zero ignition, 500 MMF capacitance, 0.005” gap setting)[195], 0.144 (24,000 voltage, RDX/acetylene black (90/10), for zero ignition, 500 MMF capacitance, 0.005” gap setting)[195], 0.256 (32,000 voltage, RDX/acetylene black (75/25), for zero ignition, 500 MMF capacitance, 0.005” gap setting)[195]

Highest energy (J) for zero ignition probability[195]:

<table>
<tr><th>Results from[195]</th><th>Bureau of Mines 1943</th><th>Bureau of Mines 1946</th><th>Bureau of Mines 1954</th><th>NOL, 1959</th></tr>
<tr><td>0.100</td><td>0.62</td><td>–</td><td>–</td><td>0.80</td></tr>
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Data from[196]:

Material	50% point energy (J)		% expl.
	3-mil foil	10-mil foil	
RDX (impact std)	0.21	0.96	0

RDX (Wabash Ground), heated explosives, data from[196]:

Temperature (°C)	50% point energy (J)		% expl.
	3-mil foil	10-mil foil	
22	0.27	1.88	8.3
75	0.18	1.05	7.7
125	0.18	0.93	23.0
175	0.10	0.37	92.0

RDX/Exon (94/6), heated molding powders, a = polystyrene holder, b = Teflon holder, data from[196]:

Temperature (°C)	50% point energy (J)		% expl.
	3-mil foil	10-mil foil	
22	0.77	1.50	50[a]
75	0.53	1.14	0[b]
125	0.45	1.01	35[b]
175	0.43	1.02	31[b]

N [%]	37.84
$\Omega(CO_2)$ [%]	−21.61
$T_{\text{phase transitions}}$ [°C]	RT, $P > 17.8$ GPa: orthorhombic (α-form) → δ-form[47], RT, P > 3.9 GPa: orthorhombic (α-form) → γ-form[47], 500 K, $P \sim 5.5$ GPa: α-form (RDX-d_6) → β-form (also known as ε-form)[47], $P < 1.5$ GPa: β-form (also known as ε-form) → α-form (RDX-d_6)[47], β-RDX → α-RDX occurs rapidly if α-RDX is present in solution[47]

Phase diagram showing the stability fields for the various polymorphs[150]: β-RDX is a metastable form[150], α-RDX (orthorhombic) is the room temperature stable orthorhombic form which undergoes a phase transition @ RT @ ~4.0 GPa with 1.6% reduction in volume (Fig. 7)[150, 191]

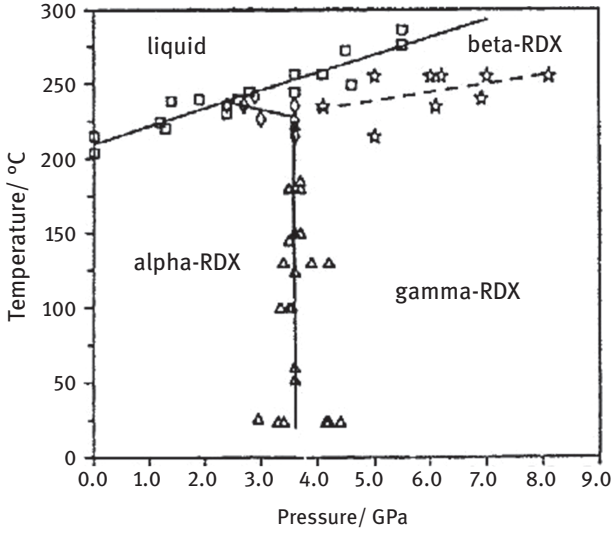

Fig. 9: Pressure versus temperature phase diagram of RDX[150].

α-phase is stable ambient orthorhombic phase, γ-phase (orthorhombic) is high-pressure phase stable > 3.8 GPa and β-phase is high-temperature-high-pressure phase stable > 2.7 GPa and 488 K and @ pressure of ~1 atm it reverts back to *α*-phase[150] (Fig. 9), α- → γ- occurs @ RT and ~3.8 GPa (reversible)[150], no dec. of γ-phase observed in pressure-temperature ranges of 1.4 <GPa <6.9 or 478 <K <508 because it always transformed to β-phase before dec. occurred[150], α- = stable, ambient orthorhombic phase[191], γ- = high pressure phase, stable >3.8 GPa[191], β- = high-temperature-high-pressure phase stable >2.7 GPa and 225 °C[191], no solid–solid phase transitions observed for α- @ atmospheric pressure – 2.5 GPa[191], α- phase melt/dec. occurs @ 215–225 °C up to 2.5 GPa[191], reversible α- → β- solid → solid phase transition between 2.5–3.8 GPa @ 225 °C[191], α- → γ- (orthorhombic) @ 3.8 GPa @ RT[191], α-/γ- phase boundary essentially *T* independent @ 3.8 GPa to 225 °C[191], >225 °C unidirectional solid/solid phase transition between γ- and β- up to 7.0 GPa[191], β- melt/dec. occurs @ 225–275 °C and 2.5–7.0 GPa[191], β- and γ- can be retrieved to ambient T @ pressure >3.8 GPa[191], @ RT β- and γ- transform to α- when pressure is decreased[191], γ- reverts to α- near 3.5 GPa[191], β- reverts to α- @ pressure near 1 atm.[191], RDX is orthorhombic and also has a very unstable polymorph which has only been isolated in very small quantities during fusion[20]

$T_{m.p.}$ [°C]	204.1 (Type I, no HMX impurities)[15, 19, 20], 192 (Type II, contains 8–12% HMX impurities)[15, 19, 20], 201[21], 203.5[27], 205 (with dec.)[29], 204[40, 61, 100, 125, 162, 164, 169, 181], 205[21, 149], 204 (with dec.)[48, 68], 205 (single crystal, nanocalorimetric curve, thermocycler @ 2,500 °C/s)[63], 200 (melting/exotherm reaction)[69], 204.1[70, 168], 202[80, 153], 203.48 (DSC @ 5 °C/min, 5 mg sample, Al pan, Al cover without crimping, under N_2, dec. occurs immediately after melting)[90], TGA/DTA (@ 1 K/min, 10 mg sample, in air, open Al pans): 198 (mpt.)[93], DSC (@ 10 °C/min, RDX after storing @ 65.5 °C for 16 weeks): 204.6 (endo peak max)[93], 204 (dec., Thomas Hoover capillary melting point apparatus @ 2 °C/min)[100], 202.83 (DSC @ 10 °C/min, 1–10 mg sample, unsealed but covered Al pans, endo)[108], 202.86 (onset, DSC, BSE HSAAP OSI (manufacturer) by NAVAIR)[130], 204.69 (endo peak max, DSC, @ 5 K/min, RDX type 1, class 1, Dyno Nobel ASA, $X_{50.3}$ = 194.5 µm)[143], 204.88 (endo peak max, DSC, @ 5 K/min, RDX type 1, class 5, Dyno Nobel ASA, $X_{50.3}$ = 17.6 µm)[143], 205.14 (endo peak max, DSC, @ 5 K/min, RS-RDX type 1, class 1, Dyno Nobel ASA, $X_{50.3}$ = 205.2 µm)[143], 203.46 (endo peak max, DSC, @ 5 K/min, RS-RDX type 1, class 5, Dyno Nobel ASA, $X_{50.3}$ = 9.7 µm)[143], 206 (endo, peak T, DSC, inert atmosphere, pierced lid)[144], 207 (endo peak T, DTA, static air atmosphere)[144], 206 (endo, peak T, DSC, inert atmosphere, open pan)[144], 205.5[154], 205.35[154], 204–206[156, 168], 204 (crystals)[159], 205[163, 168], 202–203 (type A)[19], 192–193 (type B)[19], 204.5[168], 204.5–205[172], 202 (technical product from reaction of urotropine with nitric acid fuses, corresponds to ~1% impurity present)[172], 204 (DSC @ various heating rates, closed pan)[184], 202.7[185], 478.5 K[193] † see table at end of section
$T_{b.p.}$ [°C]	dec.[70, 156], 546.3[154], 626.6 K (T_{nbp}, est., Stein–Brown method)[193]
$T_{dec.}$ [°C]	208 (DSC @ 5 °C/min), 210[4], 216[26], 219[77], 260 (@ 5 °C/s)[15], 239 (@ 10 °C/s)[15], 478 K (DTA)[7, 96], 285 (exotherm peak max., DSC @ 20 °C/min)[40], 205 (exotherm, heating rate not specified, DTA)[50], 200 (melting/exotherm reaction)[69], 210–250 (exo, DSC @ 5 °C/min, 5 mg sample, Al pan, Al cover without crimping, under N_2, dec. occurs immediately after melting)[90], 205 (dec. onset)[92], 207.84 (DSC @ 10 °C/min, 1–10 mg sample, unsealed but covered Al pans, exo, onset)[108] T_{idb} = 220.9 (@ 8 °C/min)[46], T_w = 232.2 (@ 8 °C/min)[46], T_{max} = 247.8 (@ 8 °C/min)[46], T_{idb} = 228.8 (@ 16 °C/min)[46], T_w = 245.4 (@ 16 °C/min)[46], T_{max} = 256.9 (@ 16 °C/min)[46], T_{cr} = 215–217[46], 219.5 (exo peak, DTA)[115]

	TGA/DTA (@ 1 K/min, 10 mg sample, in air, open Al pans): 145 (start of mass loss), 196 (3% mass loss), 198 (mpt.), 201 (start of exo dec.), 215 (exo peak max., DTA)[93], DSC (@ 10 °C/min, RDX after storing @ 65.5 °C for 16 weeks): 242.5 (exo peak max)[93] 233.04 (exo peak max, DSC, @ 5 K/min, RDX type 1, class 1, Dyno Nobel ASA, $X_{50.3}$ = 194.5 µm)[143], 232.85 (endo peak max, DSC, @ 5 K/min, RDX type 1, class 5, Dyno Nobel ASA, $X_{50.3}$ = 17.6 µm)[143], 234.28 (endo peak max, DSC, @ 5 K/min, RS-RDX type 1, class 1, Dyno Nobel ASA, $X_{50.3}$ = 205.2 µm)[143], 232.67 (endo peak max, DSC, @ 5 K/min, RS-RDX type 1, class 5, Dyno Nobel ASA, $X_{50.3}$ = 9.7 µm)[143], 220 (T_{onset}), 242 ($T_{inflection}$), 255 (T_{endset}) (TG-DTG, inert atmosphere, pierced lid, 98.4% dec.)[144], 244 (DSC, insert atmosphere, pierced lid)[144], 246 (exo peak *T*, DTA, static air atmosphere)[144], 216 (T_{onset}), 232 ($T_{inflection}$), 240 (T_{endset}) (exo, TG-DTG, inert atmosphere, open pan, 99.7% dec.)[144], 236 (exo, DSC, inert atmosphere, open pan)[144], 205 (DSC)[194] † see table at end of section

ρ [g cm^{-3}]	1.858 (@ 90 K, crystal), 1.841 (@ 100 K, crystal), 1.824 (@ 173 K, crystal), 1.806 (crystal)[15, 19, 26], 1.818 (@ 25 °C)[27], 1.816 (crystal)[29, 159], 1.785 (@ 298 K, gas pycnometer), 1.799[20], 1.82[11, 155, 168, 194], 1.816[67, 77], 1.85[68], 1.806[73, 92], 1.73 (pressed, 38,200 psi loading pressure, 96.0% TMD)[89], 1.81[90], 1.7881 (standard RDX, 75–355 µm fraction, Dyno Nobel)[121], 1.7919 (sieved RS-RDX, 75–355 µm fraction, Dyno Nobel)[121], 1.7761 (RS-RDX recryst. from γ-butyrolactone then sieved, 75–355 µm fraction, TNO)[121], 1.7996 ± <0.0006 (apparent crystal ρ, density gradient tube)[129], 1.125 (tap ρ, average particle size = 315.4 µm)[129], 1.126 (tap ρ, average particle size = 276.4 µm, D-RDX (ICM))[129], 0.931 (tap ρ, average particle size = 536.6 µm, C-RDX (coarse commercial RDX))[129], 1.83[149] specific gravity = 1.82 g/mL @ 20 °C[156], 1.70 (compressed to 30,000 psi)[159], 1.767 (pycnometry)[162], 1.82 (crystal)[164], 1.802 (crystal)[165], 1.83[168], 1.805[181] Loading ρ: 1.52 @ 5,000 psi[19, 29], 1.60 @ 10,000 psi[19, 29], 1.68 @ 20,000 psi[19, 29], 1.70 @ 25,000 psi[19, 29], 1.72 @ 30,000 psi[19, 29] Loading ρ: 1.46 @ 3,000 psi[164, 174], 1.52 @ 5,000 psi[164, 174], 1.60 @ 10,000 psi[164, 174], 1.63 @ 12,000 psi[174], 1.65 @ 15,000 psi[164, 174], 1.68 @ 20,000 psi[164, 174] 1.402 (Ø 4 mm, mechanically stable pellet, pressed @ 100 MPa, nanostructures RDX)[128], 1.463 (Ø 4 mm, mechanically stable pellet, pressed @ 100 MPa, nanostructured RDX)[128], sp. gr. = 1.816[172], 0.8–0.9 (gravimetric density)[172], 1.73 (on pressing @ 2,000 kg/cm^2)[172], 1.806 (X-ray data)[20], 1.799 (direct measurement @ 22.8 °C)[20]

<table>
<tr><td></td><td colspan="3">Pressed charges, pressures required will vary with particle size distribution, time under pressure and T[20]:

<table><tr><th>Pressure (psi)</th><th>ρ (g/cm^3)</th></tr><tr><td>5,000</td><td>1.52</td></tr><tr><td>10,000</td><td>1.60</td></tr><tr><td>20,000</td><td>1.68</td></tr><tr><td>30,000</td><td>1.70</td></tr></table></td></tr>
<tr><td>Heat of formation</td><td colspan="3">14.71 kg cal/mol[15, 17, 19, 26], 14.7 kcal/mol (heat of form., $\Delta H°_f$)[20], 14.69 kcal mol^{-1} (ΔH_f, crystal @ 25 °C)[27], 86.3 kJ/mol ($\Delta H_f°$)[4], 70 kJ/mol (H_f)[67], 70 kJ/mol (enthalpy of form.)[68], 18.9 kcal/mol (ΔH_f (s))[73], 60.2 kcal/mol (ΔH_f)[74], 16.7 kJ mol^{-1} (ΔH_f)[77], 70 kJ/mol[91], −70 kJ/mol[162], 301.4 kJ/kg (ΔH_f, ICT thermochemical database)[95], 70.1 kJ/mol (enthalpy of form.)[92], −96 cal/g[164], 299.7 kJ/kg (enthalpy of form.)[11], 66.0 kcal/kg (enthalpy of form.)[99], 17 ± 1.2 kcal/mol (ΔH_f^{298})[185], 15.64 kcal/mol (ΔH_f^{298})[185], 24.17 kcal/mol (ΔH_f^{298})[185], 14.7 kcal/mol ($\Delta H°_f$)[20]</td></tr>
<tr><td>Heat of combustion</td><td colspan="3">507.3 kcal/mol (@ constant volume, H_2O (l))[29], 501.8–507.3 kcal/mol (@ C^v, with H_2O (l))[19], $\Delta H°_c$ = −501.8 kcal/mol[20], 2285 kcal/kg[30, 164], ΔH_c = −9,450 kJ/kg[69], 2307.2 cal/g (@ C^p)[19], ΔQ_c = 506 ± 1.2 kcal/mol[185], ΔQ_c = 506.9 kcal/mol[185], ΔQ_c = 507.5 kcal/mol[185], ΔQ_c = 508.9 kcal/mol[185]</td></tr>
<tr><td></td><td>Calcd. (EXPLO5 6.03)</td><td>Lit. values</td><td>Exptl.</td></tr>
<tr><td>$-\Delta_{ex}U°$ [kJ kg^{-1}]</td><td>5,807</td><td>6,190[4]

1,365 kcal/kg[5]

5,647 [H_2O (l)] (ICT-code)[11, 95]

5,297 [H_2O (g)] (ICT-code)[11]

1,280 kcal/kg[30, 164]

1.50 kcal/g (Q_{max}, calcd.)[73]

5392[92]</td><td>1,370 cal/g (@ const. vol.) [H_2O (l)][29]

1.62 kcal/g [H_2O (l)][19]

1.48 kcal/g [H_2O (g)][19]

1.51 kcal/g (@ 1.7 g/cc, measured calorimetrically)[34]

6,322 [H_2O (l)] (heat of det.)[11]

1,190 kcal/kg (@ 1.100 g cm^{-3}) [H_2O vapor][99]

1,290 kcal/kg (@ 1.700 g cm^{-3}) [H_2O vapor][99]</td></tr>
</table>

		1,215 kcal/kg (@ 1.100 g cm^{-3}, calcd.) [H_2O vapor][99] 1298 kcal/kg (@ 1.700 g cm^{-3}, calcd.) [H_2O vapor][99] 1,228 cal/g (calcd.)[171]	1,320 kcal/kg (@ 1.70 g cm^{-3}, Q_{exp})[146] 1,500 cal/g (@ 1.7 g cm^{-3} loading ρ)[159] 1,320 kcal/kg[172] 2,330 cal/cm^3 (voidless, volumetric heat of explosion)[174] 2,050 cal/cm^3 (pressed @ 10,000 psi, volumetric heat of explosion)[174]
T_{ex} [K]	3,800	3,400[5] 3,425.4 (@ 1.816 g cm^{-3}, calcd. CHEETAH 6.0)[77] 4,000 (calcd., ICT-code)[95] 4,129 (@ 1.77 g cm^{-3}, ΔH_f = 14.7 kcal/mol, calcd., BKWC, THEOSTAR-T)[106] 3,349 (@ 1.77 g cm^{-3}, ΔH_f = 14.7 kcal/mol, calcd., BKWR, THEOSTAR-T)[106] 3,434 (@ 100% TMD, calcd., CHEETAH-6)[139] 2,587 (@ 1.80 g cm^{-3}, ΔH_f^0 = 639.9 kJ/kg, calcd., FORTRAN BKW)[166] 3,708 (@ 1.816 g cm^{-3}, ΔH_f = 70 kJ/mol, calcd., JAGUAR)[186] 3,220 (@ 1.80 g cm^{-3}, calcd. BKWR)[17]	2,587 (@ 1.8 g cm^{-3})[15] 3,380 °C[19, 29] 3,600 (@ 1.0 g cm^{-3})[15] 4,320 (@ 1.66 g cm^{-3})[17] 4,610 (@ 1.20 g cm^{-3})[17] 4,600 (@ 1.00 g cm^{-3})[17] 3,700 °C (@ 1.7 g cm^{-3} loading ρ)[159]

		3,260 (@ 1.77 g cm^{-3}, calcd. BKWR)[17] 3,330 (@ 1.72 g cm^{-3}, calcd. BKWR)[17] 3,400 (@ 1.66 g cm^{-3}, calcd. BKWR)[17] 3,480 (@ 1.60 g cm^{-3}, calcd. BKWR)[17] 3,630 (@ 1.46 g cm^{-3}, calcd. BKWR)[17] 3,690 (@ 1.40 g cm^{-3}, calcd. BKWR)[17] 3,780 (@ 1.29 g cm^{-3}, calcd. BKWR)[17] 3,840 (@ 1.20 g cm^{-3}, calcd. BKWR)[17] 3,890 (@ 1.10 g cm^{-3}, calcd. BKWR)[17] 3,920 (@ 1.00 g cm^{-3}, calcd. BKWR)[17] 3,920 (@ 0.95 g cm^{-3}, calcd. BKWR)[17] 4,060 (@ 0.70 g cm^{-3}, calcd. BKWR)[17] 4,180 (@ 0.56 g cm^{-3}, calcd. BKWR)[17] 4,140 (@ 1.80 g cm^{-3}, calcd. BKWS)[17] 4,160 (@ 1.77 g cm^{-3}, calcd. BKWS)[17] 4,200 (@ 1.72 g cm^{-3}, calcd. BKWS)[17] 4,230 (@ 1.66 g cm^{-3}, calcd. BKWS)[17]	

		4,280 (@ 1.60 g cm^{-3}, calcd. BKWS)[17] 4,360 (@ 1.46 g cm^{-3}, calcd. BKWS)[17] 4,390 (@ 1.40 g cm^{-3}, calcd. BKWS)[17] 4,430 (@ 1.29 g cm^{-3}, calcd. BKWS)[17] 4,460 (@ 1.20 g cm^{-3}, calcd. BKWS)[17] 4,480 (@ 1.10 g cm^{-3}, calcd. BKWS)[17] 4,490 (@ 1.00 g cm^{-3}, calcd. BKWS)[17] 4,490 (@ 0.95 g cm^{-3}, calcd. BKWS)[17] 4,450 (@ 0.70 g cm^{-3}, calcd. BKWS)[17] 4,450 (@ 0.56 g cm^{-3}, calcd. BKWS)[17]	
$p_{C\text{-}J}$ [kbar]	340	380[4] 34.47 GPa (@ 1.80 g cm^{-3}, CHEETAH 2.0)[6] 33.12 GPa (@ 1.77 g cm^{-3}, CHEETAH 2.0)[6] 340 (@ 1.767 g cm^{-3}, calcd., K-J)[57] 353 (@ 1.80 g cm^{-3}, calcd., K-J)[57] 336 (@ 1.755 g cm^{-3}, calcd., K-J)[57]	347 (@ 1.80 g cm^{-3})[15, 166] 338 (@ 1.767 g cm^{-3})[24] 388 × 10^3 atm. (@ 1.785 g cm^{-3})[30] 333.5 (@ 1.767 g cm^{-3})[15] 108 (@ 1.9 g cm^{-3})[15] 34.1 GPa (@ 1.80 g cm^{-3})[6, 17] 33.79 GPa (@ 1.77 g cm^{-3})[16, 17] 33.79 ± 0.31 GPa (@ 1.767 ± 0.011 g cm^{-3})[20]

		274 (@ 1.59 g cm^{-3}, calcd., K-J)[57]	313 (@ 1.72 g cm^{-3})[17]
			263 (@ 1.60 g cm^{-3})[17]
		211 (@ 1.40 g cm^{-3}, calcd., K-J)[57]	211 (@ 1.46 g cm^{-3})[17]
		153 (@ 1.20 g cm^{-3}, calcd., K-J)[57]	213 (@ 1.4 g cm^{-3})[17]
			166 (@ 1.29 g cm^{-3})[17]
		288 (@ 1.63 g cm^{-3}, calcd., K-J)[57]	152 (@ 1.20 g cm^{-3})[17]
		292 (@ 1.64 g cm^{-3}, calcd., K-J)[57]	122 (@ 1.10 g cm^{-3})[17]
			89 (@ 1.00 g cm^{-3})[17]
		59.9 (@ 0.7 g cm^{-3}, calcd. thermochem.)[56]	96 (@ 0.95 g cm^{-3})[17]
		108 (@ 1.0 g cm^{-3}, calcd. thermochem.)[56]	48 (@ 0.70 g cm^{-3})[17]
			32 (@ 0.56 g cm^{-3})[17]
		152 (@ 1.2 g cm^{-3}, calcd. thermochem.)[56]	12,600 kg/cm^2[19, 29]
		166.2 (@ 1.29 g cm^{-3}, calcd. thermochem.)[56]	390 (@ 1.80 g cm^{-3})[34]
			347 (@ 1.80 g cm^{-3})[34]
		209.8 (@ 1.46 g cm^{-3}, calcd. thermochem.)[56]	338 (@ 1.767 g cm^{-3})[34]
		259 (@ 1.59 g cm^{-3}, calcd. thermochem.)[56]	366 (@ 1.755 g cm^{-3})[34]
			284 (@ 1.63 g cm^{-3})[34]
		283.7 (@ 1.63 g cm^{-3}, calcd. thermochem.)[56]	287 (@ 1.59 g cm^{-3})[34]
		269 (@ 1.65 g cm^{-3}, calcd. thermochem.)[56]	196 (@ 1.44 g cm^{-3})[34]
			213 (@ 1.40 g cm^{-3})[34]
		310 (@ 1.72 g cm^{-3}, calcd. thermochem.)[56]	152 (@ 1.20 g cm^{-3})[34]
		347 (@ 1.8 g cm^{-3}, calcd. thermochem.)[56]	104 (@ 1.00 g cm^{-3})[34]
			95 (@ 1.03 g cm^{-3})[34]
		346.6 (@ 1.8 g cm^{-3}, calcd., *Mader*)[60]	195.2 (@ 1.44 g cm^{-3})[34]

		200.0 (@ 1.4 g cm^{-3}, calcd., *Mader*)[60] 34.6 GPa (@ TMD, calcd., CHEETAH 2.0)[54] 347 (@ 1.806 g cm^{-3}, calcd.)[73] 33.2 GPa (@ 1.816 g cm^{-3}, calcd. CHEETAH 6.0)[77] 360 katm (@ 1.82 g cm^{-3}, calcd., TIGER, BKW)[81] 154.1 MPa (calcd., ICT-code)[95] 32.2 GPa (@ 1.77 g cm^{-3}, $\Delta H_f = 14.7$ kcal/mol, calcd., BKWC, THEOSTAR-T)[106] 34.0 GPa (@ 1.77 g cm^{-3}, $\Delta H_f = 14.7$ kcal/mol, calcd., BKWR, THEOSTAR-T)[106] 330 (@ 100% TMD, calcd., CHEETAH-6)[139] 31.56 GPa (@ 1.767 g cm^{-3} (pycnometry density), heat of formation = −70.00 kJ/mol, Cheetah 6.0)[162] 4.443 (@ 0.69 g cm^{-3} (SSED density), heat of formation = −70.00 kJ/mol, CHEETAH 6.0)[162] 34.7 GPa (@ 1.80 g cm^{-3}; $\Delta H_f^0 = 639.9$ kJ/kg, calcd., FORTRAN BKW)[166]	338 (@ 1.767 g cm^{-3})[57] 390 (@ 1.80 g cm^{-3})[57] 366 (@ 1.755 g cm^{-3})[57] 287 (@ 1.59 g cm^{-3})[57] 213 (@ 1.40 g cm^{-3})[57] 152 (@ 1.20 g cm^{-3})[57] 283.7 (@ 1.63 g cm^{-3})[57] 269 (@ 1.64 g cm^{-3})[57] 41.5 (@ 0.7 g cm^{-3})[56] 85.5 (@ 1.0 g cm^{-3})[56] 127.4 (@ 1.2 g cm^{-3})[56] 149.7 (@ 1.29 g cm^{-3})[56] 199.6 (@ 1.46 g cm^{-3})[56] 245.8 (@ 1.59 g cm^{-3})[56] 259.9 (@ 1.63 g cm^{-3})[56] 268.6 (@ 1.65 g cm^{-3})[56] 296.0 (@ 1.72 g cm^{-3})[56] 332.1 (@ 1.8 g cm^{-3})[56] 33.9 GPa (@ 1.77 g cm^{-3})[106] 354 cal/cm^3 (voidless)[174] 257 cal/cm^3 (pressed @ 10,000 psi)[174]

		34.8 GPa (@ 1.816 g cm^{-3}, ΔH_f = 70 kJ/mol, calcd., JAGUAR)[186] 364 (@ 1.80 g cm^{-3}, calcd. BKWR)[17] 351 (@ 1.77 g cm^{-3}, calcd. BKWR)[17] 329 (@ 1.72 g cm^{-3}, calcd. BKWR)[17] 304 (@ 1.66 g cm^{-3}, calcd. BKWR)[17] 281 (@ 1.60 g cm^{-3}, calcd. BKWR)[17] 232 (@ 1.46 g cm^{-3}, calcd. BKWR)[17] 214 (@ 1.40 g cm^{-3}, calcd. BKWR)[17] 183 (@ 1.29 g cm^{-3}, calcd. BKWR)[17] 160 (@ 1.20 g cm^{-3}, calcd. BKWR)[17] 138 (@ 1.10 g cm^{-3}, calcd. BKWR)[17] 117 (@ 1.00 g cm^{-3}, calcd. BKWR)[17] 107 (@ 0.95 g cm^{-3}, calcd. BKWR)[17] 60 (@ 0.70 g cm^{-3}, calcd. BKWR)[17] 41 (@ 0.56 g cm^{-3}, calcd. BKWR)[17]	

		322 (@ 1.77 g cm^{-3}, calcd. BKWS)[17] 302 (@ 1.72 g cm^{-3}, calcd. BKWS)[17] 279 (@ 1.66 g cm^{-3}, calcd. BKWS)[17] 260 (@ 1.60 g cm^{-3}, calcd. BKWS)[17] 216 (@ 1.46 g cm^{-3}, calcd. BKWS)[17] 199 (@ 1.40 g cm^{-3}, calcd. BKWS)[17] 172 (@ 1.29 g cm^{-3}, calcd. BKWS)[17] 152 (@ 1.20 g cm^{-3}, calcd. BKWS)[17] 130 (@ 1.10 g cm^{-3}, calcd. BKWS)[17] 110 (@ 1.00 g cm^{-3}, calcd. BKWS)[17] 100 (@ 0.95 g cm^{-3}, calcd. BKWS)[17] 57 (@ 0.70 g cm^{-3}, calcd. BKWS)[17] 38 (@ 0.56 g cm^{-3}, calcd. BKWS)[17] 334 (@ 1.80 g cm^{-3}, calcd. BKWS)[17]	

VoD [m s^{-1}]	8,882 (see also [12])	8,983[4] 8,400 (@ 1.7 g cm^{-3})[5] 8,920 (@ 1.80 g cm^{-3}) (CHEETAH 2.0)[6] 8,807 (@ 1.77 g cm^{-3}) (CHEETAH 2.0)[6] 8,803 (@ TMD) (CHEETAH v8.0)[45] 8,800 (@ 1.81 g cm^{-3}, calcd., K-J)[24] 8,180 (@ 1.65 g cm^{-3}, av. value from lit.)[28] 4,989 (@ 0.7 g cm^{-3}, calcd. thermochem.)[56] 5,981 (@ 1.0 g cm^{-3}, calcd. thermochem.)[56] 6,750 (@ 1.2 g cm^{-3}, calcd. thermochem.)[56] 7,036 (@ 1.29 g cm^{-3}, calcd. thermochem.)[56] 7,626 (@ 1.46 g cm^{-3}, calcd. thermochem.)[56] 8,077 (@ 1.59 g cm^{-3}, calcd. thermochem.)[56] 8,314 (@ 1.63 g cm^{-3}, calcd. thermochem.)[56] 8,180 (@ 1.65 g cm^{-3}, calcd. thermochem.)[56] 8,528 (@ 1.72 g cm^{-3}, calcd. thermochem.)[56] 8,754 (@ 1.8 g cm^{-3}, calcd. thermochem.)[56]	8,833 8,750 8,639[6] 8,750 (@ 1.76 g cm^{-3})[11] 8,850 (@ 1.83 g cm^{-3})[13] 8,750 (@ 1.8 g cm^{-3})[17] 8,639 ± 0.041 (@ 1.767 ± 0.011 g cm^{-3})[20] 8,700 (@ 1.77 g cm^{-3})[17, 14, 58] 8,460 (@ 1.72 g cm^{-3})[17] 8,240 (@ 1.66 g cm^{-3})[17] 8,130 (@ 1.6 g cm^{-3})[17] 7,600 (@ 1.46 g cm^{-3})[17] 7,460 (@ 1.4 g cm^{-3})[17] 7,000 (@ 1.29 g cm^{-3})[17] 6,770 (@ 1.2 g cm^{-3})[17] 6,180 (@ 1.1 g cm^{-3})[17] 5,800 (@ 0.95 g cm^{-3})[17] 4,650 (@ 0.7 g cm^{-3})[17] 4,050 (@ 0.56 g cm^{-3})[17] 8,639 (@ 1.767 g cm^{-3})[15] 8,270 (@ 1.675 g cm^{-3})[28] 8,035 (@ 1.60 g cm^{-3})[15] 8,754 (@ approaching TMD)[34]

		8,950 (@ 1.83 g cm^{-3} (TMD), calcd., R-P method)[59] 8,950 (@ 1.83 g cm^{-3} (TMD), calcd., Aizenshtadt)[59] 8,890 (@ 1.83 g cm^{-3} (TMD), calcd., K-J)[59] 8,750 (@ 1.8 g cm^{-3}, calcd., *Mader*)[60] 7,310 (@ 1.4 g cm^{-3}, calcd., *Mader*)[60] 8,900 (@ TMD, calcd., CHEETAH 2.0)[54] 8,830 (@ 1.806 g cm^{-3}, calcd.)[73] 8,840 (@ 1.816 g cm^{-3}, calcd., CHEETAH 6.0)[77] 8,802 (@ 1.82 g cm^{-3}, calcd., TIGER, BKW)[81] 6,050 (@ 1 g cm^{-3}, calcd., Kamlet method)[101] 8,100 (@ 1.6 g cm^{-3}, calcd., Kamlet method)[101] 5,560 (@ 1 g cm^{-3}, calcd., Urizar method)[101] 7,990 (@ 1.6 g cm^{-3}, calcd., Urizar method)[101] 8,970 (@ 1.77 g cm^{-3}, $\Delta H_f = 14.7$ kcal/mol, calcd., BKWC, THEOSTAR-T)[106]	8,850 (LASEM method)[45] 8,833 (@TMD) (large-scale det. test)[45] 8,049 (calcd. based on 1700 g bomb sand test)[28] 6,000 (@ 1.03 g cm^{-3})[34] 7,530 (@ 1.44 g cm^{-3})[34] 8,489 (@ 1.73 g cm^{-3})[37] 4,980 (@ 0.7 g cm^{-3})[56] 5,938 (@ 1.0 g cm^{-3})[56] 6,578 (@ 1.2 g cm^{-3})[56] 6,873 (@ 1.29 g cm^{-3})[56] 7,443 (@ 1.46 g cm^{-3})[56] 7,864 (@ 1.59 g cm^{-3})[56] 8,005 (@ 1.63 g cm^{-3})[56] 8,070 (@ 1.65 g cm^{-3})[56] 8,315 (@ 1.72 g cm^{-3})[56] 8,591 (@ 1.8 g cm^{-3})[56] 8,489 (@ 1.73 g cm^{-3})[92] 6,030 (@ 1 g cm^{-3})[101] 8,110 (@ 1.6 g cm^{-3})[101] 8,640 (@ 1.77 g cm^{-3})[106] 8,390 (@ 1.650 g cm^{-3}, phlegmatized RDX (RDX/$(CH_2)_n$ 95/5), cylinder test, impulse X-ray apparatus, 300 mm long tube, 25 mm internal diameter, 2.5 mm wall thickness)[137]

		8,990 (@ 1.77 g cm^{-3}, ΔH_f = 14.7 kcal/mol, calcd., BKWR, THEOSTAR-T)[106] 8,650 (@ 1.767 g cm^{-3} (pycnometry density), heat of formation = −70.00 kJ/mol, CHEETAH 6.0)[162] 4,738 (@ 0.69 g cm^{-3} (SSED density), heat of formation = −70.00 kJ/mol, CHEETAH 6.0)[162] 8,754 (@ 1.80 g cm^{-3}, ΔH_f^0 = 639.9 kJ/kg, calcd., FORTRAN BKW)[166] 8,760 (@ 1.816 g cm^{-3}, ΔH_f = 70 kJ/mol, calcd., JAGUAR)[186] 8,770 (@ 1.80 g cm^{-3}, calcd. BKWR)[17] 8,670 (@ 1.77 g cm^{-3}, calcd. BKWR)[17] 8,500 (@ 1.72 g cm^{-3}, calcd. BKWR)[17] 8,300 (@ 1.66 g cm^{-3}, calcd. BKWR)[17] 8,100 (@ 1.60 g cm^{-3}, calcd. BKWR)[17] 7,640 (@ 1.46 g cm^{-3}, calcd. BKWR)[17] 7,450 (@ 1.40 g cm^{-3}, calcd. BKWR)[17] 7,120 (@ 1.29 g cm^{-3}, calcd. BKWR)[17]	27,000 ft/s (@ 1.6 g/mL)[153] 8,380 (@ 1.7 g cm^{-3} loading ρ)[159] 8,180 (@ 1.65 g cm^{-3}, 1.0 in charge diameter, pressed, no confinement)[164] 8,100 (@ 1.61 g cm^{-3} after 16 h @ −54 °C)[164] 8,050 (@ 1.62 g cm^{-3} after 16 h @ 21 °C)[164] 8,755 (@ 1.802 g cm^{-3})[165] 8,754 (@ 1.80 g cm^{-3})[166] 8,180 (@ 1.65 g cm^{-3})[169] 8,400 (@ 1.7 g cm^{-3})[172] 8,400 (@ 1.56 g cm^{-3})[181] 6,080 (@ 1.0 g cm^{-3})[183]

		6,860 (@ 1.20 g cm^{-3}, calcd. BKWR)[17] 6,580 (@ 1.10 g cm^{-3}, calcd. BKWR)[17] 6,320 (@ 1.00 g cm^{-3}, calcd. BKWR)[17] 6,190 (@ 0.95 g cm^{-3}, calcd. BKWR)[17] 5,360 (@ 0.70 g cm^{-3}, calcd. BKWR)[17] 4,840 (@ 0.56 g cm^{-3}, calcd. BKWR)[17] 8,960 (@ 1.80 g cm^{-3}, calcd. BKWS)[17] 8,840 (@ 1.77 g cm^{-3}, calcd. BKWS)[17] 8,630 (@ 1.72 g cm^{-3}, calcd. BKWS)[17] 8,380 (@ 1.66 g cm^{-3}, calcd. BKWS)[17] 8,150 (@ 1.60 g cm^{-3}, calcd. BKWS)[17] 7,630 (@ 1.46 g cm^{-3}, calcd. BKWS)[17] 7,420 (@ 1.40 g cm^{-3}, calcd. BKWS)[17] 7,060 (@ 1.29 g cm^{-3}, calcd. BKWS)[17] 6,790 (@ 1.20 g cm^{-3}, calcd. BKWS)[17] 6,490 (@ 1.10 g cm^{-3}, calcd. BKWS)[17]	

		6,210 (@ 1.00 g cm^{-3}, calcd. BKWS)[17] 6,060 (@ 0.95 g cm^{-3}, calcd. BKWS)[17] 5,250 (@ 0.70 g cm^{-3}, calcd. BKWS)[17] 4,720 (@ 0.56 g cm^{-3}, calcd. BKWS)[17]	
V_0 [L kg^{-1}]	793	908 (@ 0 °C)[5] 0.436 cm^3/g (@ 1.8 g cm^{-3}, calcd., *Mader*)[60] 0.523 cm^3/g (@ 1.4 g cm^{-3}, calcd., *Mader*)[60] 908[164]	903 [18] 908 (@ 0 °C and 760 mm Hg)[19, 29, 159] 700 (@ 1.5 g cm^{-3}, Dolgov's bomb) [H_2O (l)][31, 32] 890 (@ 1.5 g cm^{-3}, Dolgov's bomb) [H_2O (g)][31, 32] 910[172]

Sample name	Scan rate 20 °C/min				Scan rate 10 °C/min				Scan rate 5 °C/min				Scan rate 1 °C/min			
	Endotherm (°C)	Heat (J/G)	Exotherm (°C)	Heat (J/G)	Endotherm (°C)	Heat (J/G)	Exotherm (°C)	Heat (J/G)	Endotherm (°C)	Heat (J/G)	Exotherm (°C)	Heat (J/G)	Endotherm (°C)	Heat (J/G)	Exotherm (°C)	Heat (J/G)
SIRDX	208	46	254	3,542	206	134	242	4,796								
	206	51	253	2,503	206	167	242	4,913								
Dyno Nobel	207	136	250	5,257	202	133	242	3,706	204	95	239	4,370	204	87	240	3,327
	207	142	252	4,902									201	55	220	4,158
Holston (lot 1)	205	37	253	3,008	200	114	241	4,434								
	208	54	257	1,519												
Holston (lot 2)	208	83	250	4,515	203	87	241	4,719	202	53	238	4,486	n.d.	n.d.	219	3,520
	207	149	256	2,785	202	172	248	10,507	201	54	240	2,770	191	55	220	3,542
Holston unreprocessed	207	142	249	6,079	205	105	247	2,533	189	66	244	3,693	188	39	222	3,982
	206	91	249	5,280					192	30	242	3,663	186	49	221	4,288

† DSC of RDX samples at various scan rates[147]

<table>
<tr>
<td>Critical diameter, d_c [cm]</td>
<td>
Values from[19]:
<table>
<tr><th>RDX/wax</th><th>ρ (g/cm^3)</th><th>Critical diameter</th></tr>
<tr><td>95/5</td><td>1.05</td><td>$4.0 < d_c < 5.0$</td></tr>
<tr><td>90/10</td><td>1.10</td><td>$4.0 < d_c < 5.0$</td></tr>
<tr><td>80/20</td><td>1.25</td><td>$3.8 < d_c < 5.0$</td></tr>
<tr><td>72/28</td><td>1.39</td><td>$3.8 < d_c < 5.0$</td></tr>
</table>
Values from[87]:
<table>
<tr><th>Material</th><th>Particle size</th><th>ρ (% TMD)</th><th>d_c (mm)</th></tr>
<tr><td>RDX</td><td>25–150 µm (lightly confined in plastic tubing)</td><td>1.00 (55.4)</td><td>$1.0 < d_c < 1.15$</td></tr>
<tr><td>RDX/wax</td><td>91.8:8.2</td><td>1.695 (99.0)</td><td>< 2.2</td></tr>
</table>
Critical detonation diameter d_{c0} [mm] and specific surface area, S_g [cm^2 g^{-1}][92]:
<table>
<tr><th>S_g (cm^2 g^{-1})</th><th>d_{c0} (mm)</th></tr>
<tr><td colspan="2">Monodisperse RDX (fractions)</td></tr>
<tr><td>280 (250–350 µm)</td><td>3.78</td></tr>
<tr><td>370 (200–250 µm)</td><td>3.31</td></tr>
<tr><td>600 (90–160 µm)</td><td>2.37</td></tr>
<tr><td>1310 (0–60 µm)</td><td>1.67</td></tr>
<tr><td>9000 (3–5 µm)</td><td>0.27</td></tr>
</table>
d_{c0} (mm) @ mean crystal size (µm)[92]: 0.25 @ 3, 0.60 @ 10, 0.85 @ 20[92]
</td>
</tr>
<tr>
<td>Critical pressure of initiation of explosion</td>
<td>$P_{cr} = 0.70 \pm 0.01$ GPa (explosion initiation by impact of CL-20), $\sigma_{ult} = 82$ MPa (explosion initiation by impact of CL-20)[122], $P_{cr} = 1.10 \pm 0.03$ (commercial RDX, 10–30 µm)[140], $P_{cr} = 1.08 \pm 0.03$ (ultrafine RDX, ~1.0 µm)[140], $P_{cr} = 0.95$[146], $\sigma_{ult} = 108$ MPa[146]</td>
</tr>
</table>

<table>
<tr><td>Critical pressure [bar]</td><td>58.01 (est., Joback-Stein method)[193], 35.31 (Valderrama-Alveraz method)[193]</td></tr>
<tr><td>Critical T [°C]</td><td>217[20], 215–217 (exptl.)[124, 152], 217 (calcd.)[124, 152], 842.7 K (est., Joback-Stein method)[193], 1,112.3 K (Valderrama-Alveraz method)[193], 840 K (Maksimov)[193]</td></tr>
<tr><td>Trauzl test [cm^3, % TNT]</td><td>151–170% TNT[19], 170% TNT[28], 157–168% TNT[29], 157% TNT[164, 169], 470 cc[172], 465[182], 475[182], 480[182]</td></tr>
<tr><td>Sand test [g]</td><td>125–145% TNT[19], 123% TNT (using 200 g bomb)[29], 53.2 g sand crushed (1700 g bomb using 0.4 g sample)[28], 60.2 g (200 g bomb)[164, 169]</td></tr>
<tr><td>Koenen test [mm]</td><td>8 (≥1 explosion from 3 tests)[103]</td></tr>
<tr><td>Plate dent test</td><td>135–141% TNT[19], 7.71 mm deep crater[92], brisance = 135% TNT (@ 1.50 g cm^{-3}, method A, pressed, confined)[164]

Data from[20]:

<table>
<tr><th>Charge diameter (mm)</th><th>Density (g/cm^3)</th><th>Dent depth (mm)</th><th>Charge height (mm)</th></tr>
<tr><td>41.3</td><td>1.754</td><td>10.35</td><td>203</td></tr>
<tr><td>41.3</td><td>1.744</td><td>10.14</td><td>203</td></tr>
<tr><td>41.3</td><td>1.537</td><td>8.20</td><td>203</td></tr>
</table>
</td></tr>
<tr><td>Ballistic mortar test</td><td>150–161% TNT[19], 150% TNT[28, 164, 169]</td></tr>
<tr><td>Initiation efficiency</td><td>No detonation with No. 6 blasting cap if <14% water present[19], 0.4 g requires 0.17 g MF for detonation[80], 0.19 g MF is minimum detonating charge[164], 0.05 g LA is minimum detonating charge[164, 174]</td></tr>
<tr><td>US NOL gap test</td><td>8.20 cm gap value @ 1.640 g cm^{-3} (pressed RDX)[30, 84], 82 mm (323 cards) (50% probability point)[75]

Comparison of NOL LSGT results with those of IHE gap test, RDX-p = pressed RDX[62]:

<table>
<tr><th>Material</th><th>ρ_0 (g cm^{-3})</th><th>IHE (50% gap, in)</th><th>LSGT (in × 10^2)</th></tr>
<tr><td>RDX-p</td><td>1.64</td><td>323</td><td>285</td></tr>
</table>

No positive test @ 50 cards for a mixture of RDX 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)[170], a mixture of RDX and DMF (67% RDX by weight) gave a positive result @ 50 cards but failed @ 150 cards[170], 336 cards (RDX @ 85.1% TMD, NOL LSGT)[170], 323 cards (RDX @ 91.0% TMD, NOL LSGT)[170]</td></tr>
</table>

<table>
<tr><td>Gap test</td><td>Gap test = 12.4 kbar, charge ρ = 1.62 g cm^{-3} (RDX class E)[37],
gap test = 12.4 (class “E”) kbar @ 1.73 g cm^{-3}[92]
gap = 66 mm, Gap = 67 mm (phlegmatized RDX)[64]</td></tr>
<tr><td>LSGT [cm]</td><td>Gap$_{50}$ = 7.02 mm, L_{95} = 0.10 mm (@ 1.09 g cm^{-3})[20], Gap$_{50}$ = 6.17 mm, L_{95} = 0.01 mm (@ 1.750 g cm^{-3})[20], 67 mm (NOL)[78], 61 mm (LANL)[78]

LSGT on baseline and aged (60 °C) samples[147]:

<table><tr><td>RDX sample</td><td>baseline (kbar)
[% HMX impurities]</td><td>60 °C (kbar)</td></tr><tr><td>SIRDX
(insensitive RDX, Eurenco)</td><td>46.3
[0.0]</td><td>46.0</td></tr><tr><td>Dyno Nobel</td><td>44.3
[0.1]</td><td>45.2</td></tr><tr><td>Holston #1 (Holston RDX reprocessed, lot 1)</td><td>43.4
[2.9]</td><td>39.2</td></tr><tr><td>Holston #2 (Holston RDX reprocessed, lot 2)</td><td>41.6
[1.9]</td><td>29.1</td></tr><tr><td>Holston</td><td>35.6
34.7</td><td>[15.5]</td></tr></table>
ρ_0 = 1.53 g/cc, 85.0% TMD, 50% pressure (P_g) = 6.8 kbar[180]</td></tr>
<tr><td>SSGT [cm]</td><td>Gap$_{50}$ = 7.82 mm, L_{95} = 0.15 mm (@ 1.00 g cm^{-3})[20], Gap$_{50}$ = 8.86 mm, L_{95} = 0.15 mm (@ 1.11 g cm^{-3})[20], Gap$_{50}$ = 0.50 mm, L_{95} = – mm (@ 1.704 g cm^{-3})[20], Gap$_{50}$ = 5.18 mm, L_{95} = 0.18 mm (@ 1.735 g cm^{-3})[20], Gap$_{50}$ = 0.36 mm, L_{95} = 0.01 mm (@ 1.752 g cm^{-3})[20], 7.4 mm (NOL)[78], 4.8 mm (LANL)[78]

MRL small-scale gap test, mild steel witness block, results give the thickness of brass shim (in mm) required to attenuate a standard shock to give a 50% probability of detonation; values from[82]:

<table><tr><td rowspan="2">material</td><td colspan="3">shock sensitivity</td></tr><tr><td>ρ (% TMD)</td><td>$M_{50\%}$</td><td>std. deviation</td></tr><tr><td>RDX (250–350 µm, sieve cut)</td><td>90.00</td><td>3.76</td><td>0.12</td></tr><tr><td>RDX fine</td><td>90.04</td><td>3.79</td><td>0.15</td></tr></table>
P_{90} = 10.97 kbar (P_{90} = pressure to 90% of TMD, NSWC small-scale gap test)[98]</td></tr>
</table>

shock sensitivity, NOL SSGT (MIL-STD-1751A, Method 1042), uncoated RDX samples, samples pressed into brass cylinders @ 16,000 psi, ~1.5 g sample required per cylinder, shock sensitivity given as shock pressure necessary for 50% initiation probability[119]:

Material	Shock sensitivity (Dbg)	Shock sensitivity (kbar)	Sample ρ (g cm^{-3})	% TMD
4.8 micron RDX	5.5	19.6	1.49	81.9
Type A nano RDX	5.65 ± 0.22	20.6	1.42	78.0
Type B nano RDX	6.38 ± 0.06	26.1	1.43	78.6

Shock sensitivity of RDX pellets pressed nominally to 90% TMD (90% TMD = 1.622 g/cm^3)[126]:

RDX sample	Pellet ρ, mg/m^3 (% TMD)		Shock sensitivity (mm)†		
	Mean	Std. devi.	$M_{50\%}$	$L_{95\%}$	std. dev.
Grade A (250–300 µm sieve cut)	1.622 (90)	0.002	3.360	3.622	0.12
Grade A (125–150 µm sieve cut)	1.622 (90)	0.001	3.513	3.553–3.470	0.019
Grade A (75–106 µm sieve cut)	1.620 (89.9)	0.002	3.551	3.609–3.495	0.027
Grade E	1.623 (90.0)	0.014	3.785	4.115–3.455	0.15
Ball milled	1.624 (90.1)	0.009	3.742	3.795–3.688	0.025

RDX grade A = Albion Explosives Factory, H_2O wet supplied, dried before use; RDX grade E = Weapons Systems Research Laboratory (WSRL), H_2O wet supplied, dried before use, RDX ball-milled = nominal size 4, supplied H_2O wet by WSRL, ball-milling carried out on grade A RDX under inert solvent; †All figures are in mm of brass shim

RDX, TMD = 1.802 g cm^3, type B, class B, (2) = material loaded under vacuum[179]:

Loading pressure (kpsi)	Density (g/cm^3)		% TMD	sensitivity (DBG)			
	Avg.	*s*		Avg.	*g*	s_m	*N*
10.0	1.546	0.0035	85.8	3.250	0.0049	0.0041	43
18.3	1.618	0.0054	89.8	3.762	0.0385	0.0160	44
31	1.702	0.0084	94.5	4.413	0.0783	0.0289	46 (2)
38.2	1.717	0.0050	95.3	5.073	0.1639	0.0555	45

RDX expoding bridgewire grade[179]:

Loading pressure (kpsi)	Density (g/cm^3)		% TMD	Sensitivity (DBG)			
	Avg.	*s*		Avg.	*g*	s_m	*N*
2.0	1.188	0.0162	65.9	3.569	0.0305	0.0204	23

ρ_0 = 1.53 g/cc, 85.0% TMD, 50% pressure (P_g) = 9.3 kbar (extrapolated)[180]

Small-scale gap (booster) sensitivity test

Values from[89]:

Pressed composition	@ 93% TMD		@ 95% TMD	
	DBg	Lucite gap (mils)	DBg	Lucite gap (mils)
RDX	4.1	390	5.0	316

DBg = 30–10 log (test gap/ ref. gap)[89]

Small-scale cook-off bomb (SSCB) test

Fast cook-off (@ ~1 °C/s, pellets pressed to 90% TMD used, total mass of pellet = 20 mg, test sample = 4 × pellets of 16 mm × 16 mm): time to event = 246 s, surface *T* = 240 °C[82]

Slow cook-off (@ ~0.1 °C/s, pellets pressed to 90% TMD used, total mass of pellet = 20 mg, test sample = 4 × pellets of 16 mm × 16 mm): time to event = 1654 s, surface *T* = 218 °C[82]

Impact initiation

Critical unconfined charge thickness = 0.25 mm, critical pressure = 7000 kg/cm^2, min. impact force = 1.3 × 10^5 kg[46]

SBAT (small-scale autoignition test, Thiokol) [°C]

189[81]

5 s explosion *T* [°C]	255–260 (ignites or deflagrates only)[19, 29], 280 (type B RDX)[29], 225–235[30], fumes @ 290 but no detonation up to 360[80], 260 (dec.)[164, 174], 273 (Wood's metal bath, 40 mg)[183], 250 (extrapolated from data for 30 mg powdered sample placed in No. 8 blasting cap, Wood's metal bath)[190]
Explosion *T* [°C]	260[27], 210 (DTA/TG @ 6 °C/min)[37], 360 (with dec.)[159], 405 (0.1 sec, no cap used)[164], 316 (1 sec)[164, 174], 240 (10 s)[164, 174], 235 (15 s)[164], 405 (0.1 s)[174], 260 (dec., cook-off)[174] Temperature and time data for type 2 RDX class 1, 30 mg powdered sample placed in No. 8 blasting cap, Wood's metal bath [190]:
5 s ignition *T* [°C]	260–270 (dec.) (USA value)[30], 230–260 (dec.)(Russian value)[30], 260[102], 295 (2 s ignition T)[134]
Ignition *T* [°C]	210[54], 213[84], 215 (calorimetric)[102], 215–230[102], 220 (Wood's metal bath)[103], 222[112], 316 (1 sec, deflagrates or ignites)[19], 405 (0.1 sec, deflagrates or ignites)[19], 290 (fumes)[19]
Detonating *T* [°C]	~235[153], 260 (5 s)[169]

T (°C)	Time (s)	T (°C)	Time (s)
297	1.02	280	1.66
293	1.19	277	1.94
287	1.07	276	1.99
284	1.66	256	3.87
284	1.58	248	5.42
283	1.54	247	6.04
282	1.62	245	6.43
281	1.37	244	6.29

<table>
<tr>
<td>Thermal stability</td>
<td>
No dec. @ 65 °C after 1 year[19], no dec. @ 85 °C after 1 year[19], no dec. after 2 months @ 100 °C[19], no dec. in 8 h @ 132 °C[19], no acid and no explosion after 300 min @ 135 °C[19]

No. moles of gas/mole RDX @ 120 °C: 0 moles/22 h, 0 moles/72 h[40]
No. moles of gas/mole RDX @ 220 °C: 2.92 moles/22 h, 3.9 moles/72 h[40]
No. moles of gas/mole RDX @ 320 °C: 3.84 moles/22 h, 3.9 moles/72 h[40]

H_2O content in mass % using the Karl-Fischer method and mass loss on storage[93]:

<table>
<tr><th>sample</th><th>Storage time @ 65.5 °C</th><th>K-F value (mass %)</th><th>Mass loss after storage</th></tr>
<tr><td>RDX</td><td>None</td><td>0.09</td><td>-</td></tr>
<tr><td>RDX</td><td>4 months</td><td>0.04</td><td>0.07</td></tr>
</table>

TGA/DTA (@ 1 K/min, 10 mg sample, in air, open Al pans): 145 (start of mass loss), 196 (3% mass loss), 198 (mpt.), 201 (start of exo dec.), 215 (exo peak max., DTA)[93]

DSC (@ 10 °C/min, RDX after storing @ 65.5 °C for 16 weeks): 204.6 (endo peak max), 242.5 (exo peak max)[93]

Level of gas release during 40 h thermostating of RDX, LAVA apparatus, level of gas normalized to standard conditions[102]:

<table>
<tr><th rowspan="2">Mass of sample (g)</th><th colspan="3">Level of gas release, V (cm^3/g)</th></tr>
<tr><th>@ 100 °C</th><th>@ 120 °C</th><th>@ 150 °C</th></tr>
<tr><td>5</td><td>0.7</td><td>0.9</td><td>2.5</td></tr>
</table>

0.19% @ 120 °C, 48 h TG[115]

HPLC analysis of remaining RDX (Holston lot 1) during 200 °C thermolysis, rel. amount to standard/minutes @ 200 °C[147]: 1.00/0 min, 0.95/5, 0.80/25, 0.85/30, 0.60/180[147]

Storage for 10 months @ 85 °C causes no reduction in its stability or explosive properties[159], highly stable in long-term storage under ambient conditions[159], stored @ 85 °C for 10 months without change in stability[169], highly stable and can be stored for months @ 50 °C without dec.[172], two step mass loss: major mass loss @ 170–260 °C followed by 10% mass loss @ 240–290 °C, total mass loss ~100% (TGA, open pan)[184], single step mass loss: >95% mass loss @ 210–270 °C (TGA, pierced pan)[184]
</td>
</tr>
</table>

100 °C heat test [% mass loss] 75 °C Int. heat test [% mass loss]	0.04% mass loss in first 48 h[19, 64], 0.00% mass loss in second 48 h[19, 64], no explosions after 100 h[19, 64] 0.03% mass loss in 48 h[19, 164]
Evaporation *T* [°C]	~300 (single crystal, nanocalorimetric curve, thermal cycle @ 2,500 °C/s)[63]
LLNL reactivity test	0.02–0.025 cm^3 gas evolved[19]
Vacuum stability test [cm^3/h]	0.9 cm^3 gas evolved after 40 h @ 120 °C (5 g sample)[19], 2.5 cm^3 gas evolved after 40 h (5 g sample) @ 150 °C[19], 0.1–0.3 mL/g gas evolved after 48 h @ 120 °C[20], 3.95 cc gas evolved/5 g sample after 40 h @ 150 °C[27], 0.03 cm^3 @ 110 °C, 20 h, $\rho = 1.80$ g cm^{-3}[107, 113], 0.53 mL/5 g @ 120 °C, 48 h[115], 0.9 cm^3 gas evolved after 40 h @ 120 °C[174] @ 175 °C: 4.2 cm^3 gas evolved after 48 h[53], 15.1 cm^3 after 7 days[53] @ 150 °C: 3.2 cm^3 gas evolved after 48 h[53], 3.5 cm^3 after 21 days, 16.8 cm^3 after 28 days[53] fresh RDX: V = 0.22 mL (120 °C, 40 h)[23], aged RDX: V = 0.44 mL (120 °C, 40 h)[23] 0.2–0.6 mL/5 g (120 °C, 40 h)[26], 0.7 cc/40 h @ 100 °C[164], 0.9 cc/40 h @ 120 °C[164], 2.5 cc/40 h @ 150 °C[164]
Vapor pressure [atm. @ °C]	1.32×10^{-6} Torr @ 66 °C[52], $3.24–3.5 \times 10^{-7}$ mm Hg (@ 55.7 °C)[20], $7.14–8.6 \times 10^{-7}$ mm Hg (@ 62.6 °C)[20], $69.30–78.7 \times 10^{-7}$ mm Hg (@ 78.2 °C)[20], $667–735 \times 10^{-7}$ mm Hg (@ 97.7 °C)[20], 4.03×10^{-9} Torr @ 25 °C[149], 1.1×10^{-9} mm Hg @ 20 °C[156], 4.0×10^{-9} @ 20 °C[156], 0.0084 ppb_v (equilibrium vapor pressure @ 300 K, this value may be too low)[158], 8.2 ppb_v (equilibrium vapor pressure @ 333 K)[158], 2.1×10^3 ppb_v (equilibrium vapor pressure @ 400 K)[158], 4.0×10^{-9} mm Hg @ 25 °C[163, 168], 4.03×10^{-9} mm Hg (solid)[168], 1.00×10^{-9} mm Hg (solid)[168], 4.1×10^{-9} mm Hg (solid)[168], 1.95×10^{-9} mm Hg (solid)[168], 3.30×10^{-9} Torr @ 25 °C[188], 2.76×10^{-6} Torr @ 70 °C[188], 9.92×10^{-5} Torr @ 100 °C[188]

Values from[160]:

T (°C)	Vapor pressure (x 10^7 Torr)	Wt. loss (g × 10^3)	Time (s)	Area (cm^2)
55.7	3.50	9.63	424,080	1.355
55.7	3.24	5.05	424,080	0.766
55.7	3.42	5.06	424,080	0.728
62.6	8.21	7.63	144,900	1.351
62.6	7.14	11.54	144,900	2.35
62.6	8.63	15.02	144,900	2.53
78.2	69.3	45.09	177,300	0.791
78.2	78.7	20.79	72,000	0.791
85.3	155	53.90	57,600	1.317
97.7	735	108.48	24,120	1.355
97.7	667	55.72	24,120	0.766
97.7	702	55.68	24,120	0.728

@ RT (25 °C): 6.0 ppt (v/v) (i.e., 0.006 ppb)[55], 4.2×10^{-9} Torr @ 20 °C[70]

Values in Pa[154]: 2.84×10^{-12} (@ 15 °C)[154], 3.91×10^{-10} (@ 15 °C)[154], 7.02×10^{-11} (@ 25 °C)[154], 1.79×10^{-4} (@ 25 °C)[154], 2.42×10^{-9} (@ 25 °C)[154], 1.08×10^{-9} (@ 35 °C)[154],1.32×10^{-8} (@ 35 °C)[154], 3.58×10^{-9} (@ 40 °C)[154], 1.10×10^{-8} (@ 45 °C)[154], 6.51×10^{-8} (@ 45 °C)[154], 8.77×10^{-8} (@ 55 °C)[154], 2.90×10^{-7} (@ 55 °C)[154], 5.74×10^{-7} (@ 65 °C)[154], 1.188×10^{-6} (@ 65 °C)[154], 3.20×10^{-6} (@ 75 °C)[154], 4.47×10^{-6} (@ 15 °C)[154], 1.55×10^{-5} (@ 85 °C)[154], 1.56×10^{-5} (@ 85 °C)[154], 3.27×10^{-5} (@ 90 °C)[154], 2.85×10^{-5} (@ 90 °C)[154], 1.33×10^{-4} (@ 100 °C)[154], 9.05×10^{-5} (@ 100 °C)[154]

Values in mm Hg[154]: 3.5×10^{-7} (@ 55.7 °C)[154], 3.24×10^{-7} (@ 55.7 °C)[154], 3.42×10^{-7} (@ 55.7 °C)[154], 8.21×10^{-7} (@ 62.6 °C)[154], 7.14×10^{-7} (@ 62.6 °C)[154], 8.63×10^{-7} (@ 62.6 °C)[154], 69.3×10^{-7} (@ 78.2 °C)[154], 78.7×10^{-7} (@ 78.2 °C)[154], 155×10^{-7} (@ 85.3 °C)[154], 735×10^{-7} (@ 97.7 °C)[154], 667×10^{-7} (@ 97.7 °C)[154], 702×10^{-7} (@ 97.7 °C)[154]

Burn rate [mm/s]

Burning characteristics[104]:

Parameter	Values (*Zenin*) cited in[104]	Values (*DeLuca*) cited in [104]
ρ [g cm^{-3}]	1.67	1.67
u (linear burning rate) [mm/s]	0.5	0.48
m (mass burning rate) [kg/m^{2}s]	0.83	0.80
T_0 (initial T) [K]	293	300
T_s (surface T) [K]	593	593
Q_s (heat absorbed/evolved in condensed phase) [kJ/kg]	−0.41	−0.31

Q_m (sum of latent heat of fusion and enthalpies of polymorphic transformations of the burning surface) = 161 kJ/kg[104]
Q (enthalpy of condensed phase chemical reactions taken with the inverse sign) = 0.8 MJ/kg[104]

burn-rate characteristics[105]: pressure interval = 0.1–0.2 MPa, pressure exponent = 0.825, burn rate @ 10 MPa = 17.8 mm/s, strand ρ = 1.75 g cm^{-3}, adiabatic flame T @ 10 MPa = 3318 K[105]

burns with bright white flame in open air leaving no residue but explodes on rapid heating[172]

burning rate of RDX, 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[173]:

Explosive	Method	Loading density (g cm^{-3})	Pressure (atm.)	Apparent mass burning rate*
RDX approx. 5 µ	Paper tube	1.07	52.0	1.66 (0.8)
RDX approx. 200 µ	Paper tube	1.16	52.0	33.3 (3.9)

Mass burning rates[178]:

m, g cm^{-2} s^{-1}				
1 atm	100 atm	200 atm	400 atm	1000 atm
0.061	3.06	5.22	9.54	22.5

Burn rate and equilibrium combustion temperature[178]: $T_e = 3510$ K[178], $m = 3.06$ g cm^{-2} s^{-1} (100 atm)[178]

Dependence of burning rate on pressure, RDX, $\rho_{max} = 1.80$ g/cm^3[178]:

$\delta = \rho/\rho_{max}$	coefficients in formulae m(g cm^{-2} s^{-1}) = $a + bp^v_{atm}$			pressure (atm.)
	a	b	v	
~1.0	0.9	0.0216	1.0	100–1000
	–	0.072	0.82	10–1000

Dependence of mass burning rate on the relative density of the charge[178]:

p (atm.)	m (δ)							
1	δ	0.38	0.46	0.47	0.56	0.58	0.635	0.645
	m, g cm^{-2} s^{-1}	0.040	0.045	0.045	0.047	0.047	0.048	0.048

0.38 (@ 1 atm., SMATCH/FTIR spectroscopy)[192], 0.38 (@ 1 atm., strand burner)[192]

Pressure and temperature sensitivities of RDX burning rate @ 20 °C[135]:

p (MPa)	0.5	1	2	5	10
n	0.78	0.80	0.81	0.78	0.72
b•10^2, 1/K	0.20	0.22	0.19	0.15	0.13

Solubility [g/mL]

55 mg/L H_2O @ 25 °C[66], 42 mg/L H_2O @ 20 °C[70], almost insoluble in H_2O[79, 159], good solubility in acetone[79], insoluble in H_2O, EtOH, Et_2O, ethyl acetate, petroleum ether, CCl_4[80], very slightly soluble in hot benzene[80], soluble one part per 135 parts xylene[80], readily soluble in hot aniline, phenol, ethylbenzoate, nitrobenzene[80], moderately soluble in hot acetone (one part per eight parts acetone)[80], aqueous solubility = 60 mg/L @ 25 °C[149], moderately soluble in hot acetone[153], readily soluble in hot phenol[153], 0.060 g/L in H_2O @ 25 °C[155], 59.7 mg/L in H_2O @ 25 °C[156], practically insoluble in MeOH, EtOH, Et_2O, benzene, toluene, CCl_4 and $CHCl_3$[159], readily soluble in acetone, ethyl acetate, cyclohexanone, methyl ethyl ketone, aniline and phenol[159], 56.3 mg /L in H_2O @ 25 °C[163], 6.0 × 10^{-2} mg/mL in H_2O @ 25 °C[188]

Can be recryst. from: cyclohexanone, acetone, γ-butyrolactone, cyclohexanone/H_2O[88]; dec. after several days @ 50 °C of RDX in cyclohexanone or cyclohexanone/H_2O[88]

Approximate solubility of RDX in DMF using different methods @ different temperatures (g (RDX)/g (DMF))[145]: 0.35 (HPLC @ 22 °C), 0.40 (refractometry @ 22 °C), 0.45 (HPLC @ 40 °C), 0.50 (density method @ 40 °C), 0.55 (refractometry @ 40 °C), 0.60 (HPLC @ 60 °C), 0.65 (density method @ 60 °C), 0.70 (spectroscopy @ 60 °C), 0.75 (refractometry @ 60 °C), 0.75 (HPLC @ 80 °C), 0.78 (gravimetric @ 80 °C), 0.85 (density method @ 80 °C), 0.90 (spectroscopy @ 80 °C), 0.95 (refractometry @ 80 °C)[145]

Approximate solubility of RDX in PC (propylene carbonate) using different methods @ different temperatures (g (RDX)/g (PC))[145]: 0.075 (gravimetric @ 20 °C), 0.080 (density method @ 20 °C), 0.085 (gravimetric @ 40 °C), 0.10 (HPLC @ 40 °C), 1.1 (spectroscopy @ 40 °C), 0.16 (gravimetric @ 60 °C), 0.70 (HPLC @ 60 °C), 0.175 (spectroscopy @ 60 °C), 0.230 (gravimetric @ 80 °C), 0.275 (density method @ 80 °C), 0.275 (spectroscopy @ 80 °C), 0.285 (HPLC @ 80 °C), 0.275 (refractometry @ 80 °C)[145], 50 mg/l in H_2O[168], 42 mg/l in H_2O[168], 42.3 ± 0.6 mg/l in H_2O @ 20 °C[168], 59.9 ± 1.2 mg/l in H_2O @ 25 ± 0.2 °C[168], 59.9 ± 0.6 mg/l in H_2O @ 26.5 °C[168], 75.7 ± 1.1 mg/l in H_2O @ 30 °C[168], 60 mg/l in H_2O[168], 42.2 mg/l in H_2O[168], 50 mg/l in H_2O @ 20 °C[168], 38 mg/l in H_2O @ 20 °C[168], 42 in H_2O @ 20 °C[168], 42.3 mg/l in H_2O @ 20 °C[168], 40 mg/l in H_2O @ 20 °C[168]

Solubility in water, mg/L[154]: 26.63 (@ 15 °C)[154], 23.32 (@ 15 °C)[154], 29.67 (@ 15 °C)[154], 30.47 (@ 25 °C)[154], 40.94 (@ 25 °C)[154], 59.7 (@ 25 °C)[154], 56.35 (@ 25 °C)[154], 33.4 (@ 35 °C)[154], 55.01 (@ 35 °C)[154], 34.9 (@ 40 °C)[154], 61.57 (@ 40 °C)[154], 36.85 (@ 45 °C)[154], 41.21 (@ 55 °C)[154], 46.62 (@ 65 °C)[154], 53.24 (@ 75 °C)[154], 61.26 (@ 85 °C)[154], 65.88 (@ 90 °C)[154], 76.49 (@ 100 °C)[154]

Solubility of RDX in TNT[19]:

T (°C)	g RDX/100 g TNT
81	4.5
85	4.7
90	5.0
95	5.8
100	6.5
105	7.3
110	8.2

Crude RDX cab be recryst. from acetone or cyclohexanone after washing crude product with water[20]

Approximate values of RDX solubility, divergent values exist in the literature[19]:

Solvent	g RDX/100 g solvent						
	@ 0 °C	@ 20 °C	@ 30 °C	@ 40 °C	@ 60 °C	@ 80 °C	@ 100 °C
Acetic acid (50%)	–	–	0.12	–	0.50	1.25	–
Acetic acid (100%)	–	–	0.41	–	1.35	2.60	–
Acetic anhydride	–	4.0	4.80	6.0	9.30	–	–
Acetone	4.2	6.8	8.40	10.3	15.3	–	–
Acetonitrile	–	–	12.0	16.2	24.6	33.0	–
Alcohol, ethyl	0.04	0.10	–	0.24	0.60	1.20	–
Benzene	–	0.05	0.06	0.09	0.20	0.40	–
CCl_4	0.0013	0.0022	0.0034	0.007	–	–	–
Chlorobenzene	0.20	0.33	0.44	0.56	–	–	–
$CHCl_3$	–	0.015	–	–	–	–	–
Cyclohexanone	–	12.8 (@ 25 °C)	–	–	–	–	25 (@ 97 °C)
Cyclopentanone	–	–	11.5 (@ 28 °C)	–	–	–	37 (@ 90 °C)
DMF	–	25.5	27.3	29.1	33.3	37.7	42.6
Ether, diethyl	–	0.055	0.075	–	–	–	–
Beta-ethoxyethyl acetate	–	1.48	1.55	1.9	3.4	–	–
Isoamyl alcohol	–	0.026	0.04	0.06	0.21	0.50	1.33
Methanol	–	0.235	0.325	0.48	1.06	–	–
Methyl acetate	–	2.95	3.30	4.10	6.05 (@ 52 °C)	–	–
Toluene	–	0.02	0.025	0.05	0.125	0.295	0.64
Trichloroethylene	–	0.20	0.21	0.22	0.23 (@ 52 °C)	–	–
TNT	–	–	–	–	–	4.4	7.0
Water	–	0.005	–	0.25 (@ 50 °C)	–	–	0.28

Solubility of RDX (g/100 g solvent) after 5 min stirring[170]:

Solvent	25 °C	40 °C	60 °C	80 °C	98 °C
DMSO	41	51	66	87	113
DMF	37	45	58	76	96
N-Methylpyrrolidone	40	47	58	72	84
Butyrolactone	14		28	41	61
Dimethylacetamide	33				
Acetone	8.2	12	17		
Cyclohexanone	7.7		15	23	33
Acetonitrile	5.5	8.8	14	26	
Cyclopentanone					38
Hexamethylphosphoramide	16				45
Aniline	1.9				

Solubilities in binary solvent mixtures @ 25 °C (g RDX/100 g solvent) after 5 min stirring[170]:

Solvent	g RDX/100 g solvent
DMSO	41
NMP	40
NMP 79.2% DMSO 20.8%	41
DMF	37
DMF 71.7% DMSO 28.3%	39
Butyrolactone	14

Solubility of RDX in DMF (g RDX/100 g solvent) after 5 min stirring[170]:

@ 0 °C	@ 25 °C	@ 60 °C	@ 80 °C	@ 98 °C
27	37	58	76	96

Comparison of solubilities (g/100 g) after 5 min and 30 min stirring @ 25 °C[170]:

Solvent	After 5 min stirring	After 30 min stirring
DMSO	41	41
DMF	37	36
Acetonitrile	5.5	5.5

Poorly soluble in water, Et_2O, EtOH, $CHCl_3$ and dil. nitric acid[172], readily soluble in acetone and conc. nitric acid[172]

Solubility data from[172]:

Solvent	*T* (°C)	Solubility (g/100 g solvent)
Water	15	0.01
	100	0.15
Acetone	20	7.413
	53	17.50
EtOH	20	0.104
MeOH	21	0.187
Benzene	21	0.015
Toluene	18	0.032
Chloroform	20	0.008
Anhydrous ether	20	0.038
CS_2 and CCl_4	18	does not dissolve
Cyclohexane	25	12.7
	97	27.0
Nitrobenzene	25	1.5
	97	12.4

Data from[172]:

HNO_3 concentration (%)	Hexogen solubility (%)
93	12.5
80	2.2
70	0.44
60	Traces

Data from[172]:

T (°C)	30	40	60	80	95	106	135	140	154
Solubility in aniline (%)	0.40		2.55	3.65	4.20		4.74		5.12
Solubility in mononitrotoluene (%)		1.93	3.81		9.03	12.22	27.4	29.43	

Solubilities @ 25 °C and 100 °C[172]:

T (°C)	Solvent						
	Cellosolve	Methyl-cellosolve	Carbitol	Methyl-carbitol	Acetate-carbitol	Butyl-carbitol	DMF
25	1.6	2.8	2.6	3.1	1.5	1.6	31.9
100	9.3	13.3	10.0	13.5	7.9	6.4	71.1

56.35×10^{-3} g/L in H_2O[193], 14.2×10^{-3} g/L in H_2O @ 298.15 K (est., *Klopman*)[193], 12.6×10^{-3} g/L in H_2O @ 298.15 K (est., COSMOtherm)[193]

g RDX/100 g solvent @ various temperatures, data from[20]:

Solvent	@ 20 °C	@ 40 °C	@ 60 °C
99.6% acetic acid	0.46	0.56	1.22
71.0% acetic acid	0.22	0.37	0.74
Acetone	6.81	10.34	–
Isoamyl alcohol	0.026	0.060	0.210
Benzene	0.045	0.085	0.195
Chlorobenzene	0.33	0.554	–
Cyclohexanone	4.94	9.20	13.9
DMF	–	41.5	60.6
EtOH	0.12	0.24	0.58
Methyl acetate	2.9	4.1	–
Methylcyclohexanone	6.81	10.34	–
Methyl ethyl ketone	3.23	–	–
Toluene	0.020	0.050	0.125
Trichloroethylene	0.20	0.24	–
Water	0.005	0.0127	0.03

<table>
<tr><td>Hygroscopicity</td><td>Nonhygroscopic[153, 172], non-hygroscopic (pure compound)[159], 0.02% @ 25 °C with 100% RH[164], non-hygroscopic @ 30 °C and 90% RH[169]</td></tr>
<tr><td>Photosensitivity</td><td>Aqueous RDX solutions before and after UV irradiation in continuous flow system as determined by LC and TLC[72]:

<table>
<tr><th>UV exposure time (h)</th><th>LC RDX (ppm)</th><th>pH</th><th>TLC detectable products</th></tr>
<tr><td>0</td><td>45.5</td><td>5.8</td><td>RDX</td></tr>
<tr><td>2</td><td>0</td><td>3.8</td><td>0</td></tr>
<tr><td>4</td><td>0</td><td>3.6</td><td>0</td></tr>
<tr><td>6</td><td>0</td><td>3.5</td><td>0</td></tr>
<tr><td>24</td><td>0</td><td>3.4</td><td>0</td></tr>
</table>

UV – 0.1% H_2O_2 static system treatment of aqueous RDX solutions[72]:

<table>
<tr><th>UV exposure time (h)</th><th>ppm H_2O_2</th><th>TOC analyzer</th></tr>
<tr><td>0</td><td>1000</td><td>12.8</td></tr>
<tr><td>0.5 > 5, < 100</td><td>2.37</td><td></td></tr>
<tr><td>2.5 ~ 3</td><td>-</td><td></td></tr>
<tr><td>3.0</td><td>0</td><td>-</td></tr>
</table>

RDX is readily degraded photochemically[149], aqueous solns. of RDX are photolyzed slowly by sunlight[149], phototransformation of RDX is the primary physical mechanism that degrades RDX in aqueous solns.[156], phototransformation in soil is not significant[156]</td></tr>
<tr><td>Radiation sensitivity</td><td>Does not show extremely high resistance, but shows moderate resistance after exposure to γ-rays with intensity of 3×10^4 Roentgens/h administering doses of 20 megaroentgens with respect to chemical stability and shows quite high chemical stability if the doses are <5 megaroentgens (cobalt-60 source)[159], unaffected by solar radiation[172]

RDX irradiated at ambient T using 0.41 MeV $^{198}_{79}$Au γ-rays; volumes of gas produced measured during and after irradiation, amount of gas evolved as function of gamma dose[199]:

<table>
<tr><th>gamma energy absorbed, 10^7 R</th><th>gas evolved (mL/g) @ STP</th></tr>
<tr><td>1</td><td>0.2</td></tr>
<tr><td>2</td><td>0.5</td></tr>
<tr><td>3</td><td>1</td></tr>
<tr><td>4</td><td>1.5</td></tr>
</table>
</td></tr>
</table>

Critical doses and *T* to initiate RDX by pulsed high-energy electrons, [a] = estimated 50% initiation dose[199]:

Explosive	Critical dose (J/g)		ignition *T* (°C)	
	Calcd.	Exptl.[A]	Calcd.	Exptl.
RDX	1.61	> 167	300	229–260

Data from[201]:

Exposure rate (R/h)	Total dose (R)	Vacuum stability test	
		100 °C (cc/g/40 h)	200 °C (cc/2 g/2 h)
6.4×10^5	control	0.09	
	1.0×10^7	0.91	Deflagrated (10 min)
	9.0×10^7	11 + (16 h)	Deflagrated (12 min)
	1.0×10^9	Material stuck in vial	

DTA for irradiated RDX @ 20 °C/min[201]:

Total dose (R)	Endotherms				Exotherms				Comments
	1st		2nd		1st		2nd		
	Onset (°C)	Peak (°C)	Onset (°C)	Peak (°C)	Onset (°C)	Peak (°C)	Onset (°C)	Peak (°C)	
0	180	193		197	204	250			Decomp. dip
1.0×10^7	180	194			206	252			
9.0×10^7	175	184	190	194	205	251			Decomp. dip
1.06×10^9	170	190			200	258			

TGA for irradiated RDX[201]:

Total dose (R)	Heating rate (°C/min)	Weight (mg)	Start of dec (°C)	10% weight loss *T* (°C)	Total weight loss (%)	Remarks
0	20	8.9	190	230	14 @ 240 °C	Deflagrated @ 240 °C
1.0×10^7	20	8.4	160	224	23 @ 240 °C	Deflagrated @ 240 °C
9.0×10^7	20	8.6	38	63	40 @ 240 °C	Deflagrated @ 240 °C

Effect of gamma radiation on the mpt. and color[201]:

Total dose (R)	Mpt. (°C)	Color
0	197.5	White
1.0×10^7	198	White
9.0×10^7	203	White
1.06×10^9	191 (Dec.)	White paste

IS for irradiated explosives, 50% fire height in inches, Bruceton method (P.A. apparatus, 2 kg mass)[201]:

Total Co^{60} gamma dose (R)	$\bar{X}$ mean (in)	σ std. dev. (in)
0	14.75	3.86
1.0×10^7	14.30	0.63
9.0×10^7	11.50	0.76

Effect of gamma radiation on explosion *T* (5 s explosion *T* in °C) and activation energy (kcal/mol)[201]:

Total dose (R)	5 s explosion *T* (°C)	Apparent activation energy (kcal/mol)
0	261	14.15
9.0×10^7	249	14.61

Effect of gamma radiation on rates of detonation[201]:

Total dose (R)	Density (g/cc)	Density after irradiation (g/cc)	Rate of detonation (m/sec)	Detonation pressure (kbar)
0	1.69	–	8,380	297
1.0×10^7	1.70	1.68	8,360	294
1.0×10^8	1.70	Very fragile	6,935	–
1.0×10^9	Pellets crumbled			

Data obtained after exposure to gamma radiation[174]:

Weight of sample (g)	5
Vol. of gas produced (mL/g) in following times (days)	
10	0.16
20	0.44
30	0.87
40	1.49
50	–
90	–
Total irradiation time (days)	44
Purity of sample by chemical analysis (%)	
Original material	–
Irradiated material	–
Melting points, corrected (°C)	
Original material	204.8
Irradiated material	204.8
IS (P.A. apparatus) (in)	
Original material	9
Irradiated material	8
IS (B.M. apparatus, 2 kg mass) (cm)	
Original material	40
Irradiated material	25

	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: 61.7 Irradiated material: 62.0
Compatibility	Slowly hydrolyzed by boiling dil. sulfuric acid or sodium hydroxide[19], slow dec. in conc. sulfuric acid if allowed to stand[19], no dec. by hot or cold dil. HCl[19], dec. on heating RDX with $Ca(OH)_2$ (equal parts) @ 60 °C for 4 h[19], forms unstable compounds if mixed with heavy metal oxides such as those of Cu or Fe[19], no corrosion of Ni or Zn with dry RDX[19], slight corrosion of Zn and Ni if 0.5% moisture present[19], dry or moist RDX causes very slight corrosion of Cu, brass, mild steel or Cd[19], dec. after several days @ 50 °C of RDX in cyclohexanone or cyclohexanone/H_2O[88] VST @ 110 °C, 20 h: RDX = 0.03 cm^3 (ρ = 1.80 g cm^{-3})[107], RDX/TNT (60/40) = 0.13 cm^3 (ρ = 1.72 g cm^{-3}, 99.0% TMD)[107, 113], RDX/TNAZ (60/40) = 0.10 cm^3 (ρ = 1.78 g cm^{-3}, 98.0% TMD)[107, 113] Not affected by moisture[153], slightly reacts with copper-plated steel[153], mixtures of RDX with copper oxides or iron oxides may ignite @ T>212 °C[153], doesn't react with common metals or nitric acid[153], dry RDX causes no corrosion of metals, in the presence of moisture only slight corrosion of metals occurs[159], doesn't react with Al or stainless steel[169], slightly reacts with Cu, brass, mild steel and Cd[169], reacts slightly with Ni and Zn when damp[169], doesn't react with dil. acid[172], reacts with conc. sulfuric acid[172], hydrolyzes in alkali dissolved in aqueous acetone[172] RDX compatibility data, 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[174]:

<table>
<tr><td></td><td>
<table>
<tr><th>Material</th><th>Compatibility</th><th>Material</th><th>Compatibility</th></tr>
<tr><td>Mg</td><td>A, N, VS</td><td>Cu plated steel</td><td>B, VS, VS</td></tr>
<tr><td>Al</td><td>A</td><td>Ni plated steel</td><td>A, N, S</td></tr>
<tr><td>Zn</td><td></td><td>Zn plated steel</td><td>A, N, S</td></tr>
<tr><td>Fe</td><td>A</td><td>Sn plated steel</td><td>A</td></tr>
<tr><td>Steel</td><td>A, VS, S</td><td>Magnesium aluminum</td><td></td></tr>
<tr><td>Sn</td><td>A</td><td>Monel metal</td><td></td></tr>
<tr><td>Cd</td><td></td><td>Brass</td><td>A, S, S</td></tr>
<tr><td>Cu</td><td>A, S, S</td><td>Bronze</td><td>A</td></tr>
<tr><td>Ni</td><td>A</td><td>18–8 stainless steel</td><td>A, N</td></tr>
<tr><td>Pb</td><td>A</td><td>T</td><td>N</td></tr>
<tr><td>Cd plated steel</td><td>VS, VS</td><td>Silver</td><td>N</td></tr>
</table>
</td></tr>
<tr><td>Heat of sublimation [kJ/mol]</td><td>31.1 kcal/mol (latent heat of sublimation)[20], 128[71], 31.11 kcal (molar heat of sublimation)[160], 140.0 cal/g (specific heat of sublimation)[160], 130 kJ/mol[184]</td></tr>
<tr><td>Activation energy for dec. [kcal/mol]</td><td>48 (T interval 210–250 °C, calcd. using the ASTM method)[103]</td></tr>
<tr><td>Heat conductivity, λ [W/(mK)]</td><td>0.25[104], 2.53×10^{-4} cal $cm^{-1}s^{-1}$ °C^{-1} @ RT (Rogers)[125], 7×10^{-4} cal $cm^{-1}s^{-1}$ °C^{-1} (Zinn)[125], 6.22×10^{-4} cal $cm^{-1}s^{-1}$ °C^{-1}[125]</td></tr>
<tr><td>Thermal conductivity [cal/sec/cm/°C]</td><td>6.91×10^{-4} @ 1.263 g cm^{-3}[164], 6.98×10^{-4} @ 1.533 g cm^{-3}[164]</td></tr>
<tr><td>Specific heat</td><td>0.26×10^{-4} cal g^{-1} °C^{-1} (@ RT)[125], 0.24×10^{-4} cal g^{-1} °C^{-1}[125], 0.30 kcal/g°C[172]

Values in cal/g/°C[19, 164]:

<table>
<tr><th>T (°C)</th><th>Specific heat (cal/g/°C)</th><th>T (°C)</th><th>Specific heat (cal/g/°C)</th></tr>
<tr><td>20</td><td>0.298</td><td>100</td><td>0.406</td></tr>
<tr><td>40</td><td>0.331</td><td>120</td><td>0.427</td></tr>
<tr><td>60</td><td>0.360</td><td>140</td><td>0.446</td></tr>
<tr><td>80</td><td>0.384</td><td></td><td></td></tr>
</table>
</td></tr>
</table>

Latent heat of fusion [cal g^{-1}]	35.5 cal/g (latent heat of melting)[20], 38.4[125]
Rifle bullet impact tests	More sensitive than Tetryl[159], 100% explosions in trials[164, 174]
Bourdon manometer [mL/g]	0.22 @ 120 °C, 48 h[115]
Pressing loads required to form pellets of 90% TMD	250–300 µm sieve cut requires 1260 kg (76.6 MPa)[126], 125–150 µm sieve cut requires 1,520 kg (92.4 MPa)[126], 75–106 µm sieve cut requires 1,700 kg (103.3 MPa)[126], grade E RDX requires 1000 kg (60.8 MPa)[126], ball-milled requires 350 kg (21.3 MPa)[126] (*RDX grade E = Weapons Systems Research Laboratory (WSRL), H_2O wet supplied, dried before use, RDX ball-milled = nominal size 4, supplied H_2O wet by WSRL*)[126]
Gurney energy [kJ/kg]	3,734 (@ 1.650 g cm^{-3}, phlegmatized RDX (RDX/$(CH_2)_n$ 95/5), cylinder test, impulse X-ray apparatus, 300 mm long tube, 25 mm internal diameter, 2.5 mm wall thickness)[137]
Gurney velocity [m/s]	2,733 (@ 1.650 g cm^{-3}, phlegmatized RDX (RDX/$(CH_2)_n$ 95/5), cylinder test, impulse X-ray apparatus, 300 mm long tube, 25 mm internal diameter, 2.5 mm wall thickness)[137]
$\Delta H_{melting}$ [J g^{-1}]	65.9 (DSC, endo peak, inert atmosphere, pierced lid)[144], 140.5 (DSC, endo peak, inert atmosphere, open pan)[144], 36 kJ/mol[184], 39.52 kJ/mol (est.)[193], 37.66 kJ/mol[193]
Heat of fusion [cal/g]	38.26[149], 32.86[149]
ΔH_{dec} [J g^{-1}]	988 (DSC, exo peak, inert atmosphere, pierced lid)[144], 543 (DSC, exo peak, inert atmosphere, open pan)[144], 860 cal/g (est.)[171], 2,250 (DSC, closed pan)[184]
ΔH_{vap} [kcal/mol]	35.02 (@ 25 °C)[154], 94 kJ/mol (est. based on heats of sublimation and fusion)[184], 127.1 kJ/mol[188]
Heat of crystallization [kcal/mol]	21.3[172]
Diffusion coefficient (air) [cm^2/s]	0.074 (air)[149, 168], 0.0931 (air)[168], 7.15×10^{-6} (water)[149, 168], 8.87×10^{-6} (water)[168]
Log K_{ow}	0.87[149, 156, 188, 193], 0.81[149], 0.86[149], 0.13 (@ 15 °C)[154], 0.917 (@ 15 °C)[154], 0.39 (@ 25 °C)[154], 0.89 (@ 25 °C)[154], 0.87 (@ 25 °C)[154], 0.64 (@ 35 °C)[154], 0.864 (@ 35 °C)[154], 0.75 (@ 40 °C)[154], 0.855 (@ 40 °C)[154], 0.85 (@ 45 °C)[154], 1.03 (@ 55 °C)[154], 1.19 (@ 65 °C)[154], 1.33 (@ 75 °C)[154], 1.44 (@ 85 °C)[154], 1.49 (@ 90 °C)[154], 1.58 (@ 100 °C)[154], 0.87 (@ 25 °C)[155], 0.81–0.87 (@ 25 °C)[155], 0.90[163, 193], $K_{ow} = 8.7 \pm 0.28$ l/kg[168], $K_{ow} = 7.2$ L/kg[168], $K_{ow} = 8.1$ L/kg[168], $K_{ow} = 8.6$ L/kg[168], $K_{ow} = 8.7$ L/kg[168], $K_{ow} = 0.86$ l/kg[168], $K_{ow} = 7.41$[188], 0.85 (@ 298.15 K, Broto method)[193], 1.04 (@ 298.15 K, Ghose method)[193], 0.90 (@ 298.15 K, COSMOtherm method)[193]

<table>
<tr><td>Log K_{oc}</td><td>2.00[149, 188], 1.80[156], K_{oc} = 2.00 L/kg[168], K_{oc} = 2.13 L/kg[168], K_{oc} = 0.89, 1.87, 2.43 l/kg[168], K_{oc} = 1.62, 2.10 L/kg[168], K_{oc} = 420 L/kg[168], K_{oc} = 0.8–4.2 L/kg[168], K_{oc} = 100[188]</td></tr>
<tr><td>Biodegradability</td><td>Strongly resists biodegradation[149], RDX migrates slowly in soils[149], biodegrades very slowly under aerobic conditions[156], biodegradability soil (aerobic) = negligible[168], biodegradability soil (anaerobic) = significant co-metabolism[168]</td></tr>
<tr><td>Half-life in soil [days]</td><td>13,140[168], 2.52 × 10^{6}[168], 0.17–0.25[168], 323–3900[168]</td></tr>
<tr><td>Half-life in water [days]</td><td>6.62[168], 85,045[168], 7[168], 3.21 @ 250 mV[168], 9 × 10^{6}[168]</td></tr>
<tr><td>Fracture surface energy [J m^{-2}]</td><td>0.11 and 0.07 for two cleavage planes[161]</td></tr>
<tr><td>Hardness</td><td>24.1 kg mm^{-2} (Vickers)[161], 2.5 (Moh’s scale, scratch hardness)[19], 2.5 (Moh’s)[164], 24.1 ± 0.8 kg mm^{-2} (single crystals, ~5 mm diameter, @ 20 °C, Vicker’s hardness)[167]</td></tr>
<tr><td>Small-scale explosivity device (SSED)</td><td>British.303 cartridge, 2 g explosive, RP-3 EBW[162]:
<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>30</td><td>1.07</td><td>11.3428</td><td>1.4285</td><td>12.6</td></tr>
<tr><td>30</td><td>1.07</td><td>11.208</td><td>1.3939</td><td>12.4</td></tr>
<tr><td>30</td><td>1.07</td><td>11.1956</td><td>1.1714</td><td>10.5</td></tr>
</table></td></tr>
<tr><td>Plate cutting test</td><td>Brisance = 125% TNT[19]</td></tr>
<tr><td>Fragmentation test</td><td>Brisance = 141% TNT (51 g RDX, ρ = 1.50 g cm^{-3}, 40 mm shell)[19]</td></tr>
<tr><td>82.2 °C KI test</td><td>60 min[19]</td></tr>
<tr><td>Abel test</td><td>Withstands >60 h @ 60 °C[172]</td></tr>
<tr><td>Flash point [°C]</td><td>230[172]</td></tr>
</table>

<table>
<tr><td>Laser ignition</td><td>Successful detonation, if RDX sample compressed against glass plate (Ruby laser (6943 Å) both in free running and Q-switch modes)[174]

Detonation conditions using laser-produced heat and shock[177]:

<table>
<tr><th>ρ or pressing force (g/cc)</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 (µs)</th><th>Laser type</th><th>Pulse duration (µs)</th></tr>
<tr><td>1.18</td><td>Confined</td><td>694</td><td>< 3,000</td><td>1</td><td>3.98</td><td>Q-switced ruby</td><td>0.10</td></tr>
<tr><td>1.18</td><td>Confined</td><td>694</td><td>< 3,000</td><td>3.5</td><td>4.90</td><td>Q-switched ruby</td><td>0.25</td></tr>
<tr><td>1.52</td><td>Confined</td><td>694</td><td>< 3,000</td><td>3.8</td><td>3.62</td><td>Q-switched ruby</td><td>0.72</td></tr>
</table></td></tr>
<tr><td>Critical air gap</td><td>0.318 in (0.2 in diameter)[174], 0.144 in (0.2 inch diameter, RDX/calcium stearate, 98.0/2.0)[174]</td></tr>
<tr><td>Critical Lucite gap</td><td>50% gap, 0.470 in, $DB_g = 3.28$ (donor = RDX, 1 in long, 0.2 in diameter, pressed in steel @ 10 kpsi)[174], 50% gap, 0.392 in, 4.07 DB_g (RDX/calcium stearate (99.3/0.7) donor = RDX, 1 in long, 0.2 in diameter, pressed in steel @ 10 kpsi)[174], 50% gap, 0.332 in, 4.79 DB_g (RDX/calcium stearate (98.6/1.4) donor = RDX, 1 in long, 0.2 in diameter, pressed in steel @ 10 kpsi)[174], 50% gap, 0.313 in, 5.04 DB_g (RDX/calcium stearate (98.0/2.0) donor = RDX, 1 in long, 0.2 in diameter, pressed in steel @ 10 kpsi)[174], 50% gap, 0.299 in, 5.25 DB_g (RDX/calcium stearate (97.2/2.8) donor = RDX, 1 in long, 0.2 in diameter, pressed in steel @ 10 kpsi)[174]</td></tr>
<tr><td>Small scale Lucite gap test</td><td>RDX @ 1.5649 g cm^{-3} loading ρ, loading pressure = 10.0 kpsi, sensitivity = 3.283 DB_g[174], RDX @ 1.7373 g cm^{-3} loading ρ, loading pressure = 38.2 kpsi, sensitivity = 5.069 DB_g[174]</td></tr>
<tr><td>Reflectance tests</td><td>Reflectance tests @ 10,600 Å (continuous wave yttrium garnet aluminum laser, pressed explosive)[176]:

<table>
<tr><th>Particle size, mesh</th><th>Loading pressure (10^3 psi)</th><th>Reflectance, %</th></tr>
<tr><td>Through 325</td><td>10</td><td>80.3</td></tr>
<tr><td>Through 60–100</td><td>50</td><td>73.6</td></tr>
</table></td></tr>
<tr><td>Combustion T [K]</td><td>Burn rate and equilibrium combustion temperature[178]: $T_e = 3510$ K[178], $m = 3.06$ g cm^{-2} sec^{-1} (100 atm.)[178]</td></tr>
</table>

Small-scale shock reactivity test (SSRT)	Used sample weight = 504 mg, dent = 589 mg SiO_2[197]
Gun propellant characteristics	Impetus = 1403 J/g[67], flame temperature = 4122 K[67]

VoD calculated using various methods[29]:

Kistiakowsky	5,380 m/s @ 1.0 g cm^{-3}[29], 8,000 m/s @ 1.60 g cm^{-3}[29]
Kast	8,370 m/s @ 1.70 g cm^{-3} (cylindrical charge, 13.6 mm diameter, 75 mm long)[29], 8360 m/s @ 1.67 g cm^{-3}[29]
Tonegutti	7,890 m/s @ 1.56 g cm^{-3} (charge diameter = 25 mm)[29], 8210–8,225 m/s @ 1.60 g cm^{-3}[29]
Evans	8,250 m/s @ 1.60 g cm^{-3}[29]
Vivas	8,380 m/s @ 1.70 g cm^{-3}[29]
Pérez-Ara	max. VoD for RDX = 8,500 m/s[29]
Unspecified	8,570 @ 1.80 g cm^{-3} with pressure = 341 kbar and temperature of explosion = 2,668 K[30]

Luminosity method (exptl./eqn. combination): 8,800 m/s @ 1.79 g cm^{-3}, T = 3700 K, Pressure = 390,000 atm.[30]

VoD after storage, charges of sticks of $1–1/8$ in diameter and 18 in long, drum camera apparatus[30]:
RDX pellets, storage 16 h @ -65°F, ρ = 1.61 g cm^{-3}, VoD = 8,100 m/s[30]
RDX pellets, storage 16 h @ + 70°F, ρ = 1.62 g cm^{-3}, VoD = 8,050 m/s[30]

RDX burning characteristics:
RDX combustion parameters, sub-atmospheric, atmospheric and high pressure @ $T_0 = 20$ °C[135]:

p (MPa)	0.05	0.075	0.1	20	30
m (g/cm^{2}c)	0.03	0.05	0.08	4.1	4.9
T_s (°C)	273	296	318	561	571
$(dT/dx)_0 \bullet 10^{-4}$ (K/cm)	6.3	7	10	36	41
q (cal/g)	242	165	152	14	14
q_r (cal/g)	5	4.8	6	5	4
Q (cal/g)	−116	−30	−10	226	232
l (mkm)	400	270	190	19	17
l_m (mkm)	200	170	130	20	18
ks$\bullet 10^{-4}$ (cal/cm•K•s)	5	5	6	31	33
T_f (°C)	1,600	1,800	2,100	2,870	2,875
L (mm)	1.0	1.5	1.0	0.15	0.13
l_R (mkm)	20.6	16.4	12.7	1.7	1.5
d (mkm)	200	130	80	2.0	1.7
L/d	5	12	13	75	76
W	0	0.23	0.3	0.96	0.98
F_s (kcal/cm^{3}s)	−1.6	−0.7	−0.013	5870	8,080
F_0 (kcal/cm^{3}s)	3.2	–	3.5	550	850

RDX combustion parameters[135]:

p (MPa)	0.5		1			2			5			10		
T_0 (°C)	20	100	−100	20	100	−100	20	100	−100	20	100	−100	20	100
m (g/cm^{2}c)	0.28	0.35	0.40	0.48	0.6	0.7	0.84	1.0	1.54	1.76	2.0	2.48	2.88	3.2
T_s (°C)	389	403	412	424	441	452	465	479	509	517	521	533	541	547
$(dT/dx)_0 \bullet 10^{-4}$ (K/cm)	15	12	22	20	15	24	22	18	28	25	22	31	28	25
q (cal/g)	70	46	25	58	36	50	38	27	28	22	17	20	16	13
q_r (cal/g)	11	9	13	11	9	12	11	9	11	9	7	8	7	6
Q (cal/g)	94	95	145	122	120	188	158	145	234	197	173	254	215	190
l (mkm)	80	100	55	60	70	35	40	55	25	30	40	18	20	30
l_m (mkm)	70	95	35	50	80	30	35	60	20	30	50	16	20	35
$k_s \bullet 10^{-4}$ (cal/cm•K•s)	9	16	9	12	17	10	13	22	15	13	32	18	23	38
T_f (°C)	2,500	2,550	2,500	2,600	2,700	2,600	2,700	2,800	2,700	2,820	2,300	2,750	2,860	2,950
L (mm)	1.25	1.3	1.0	1.3	1.4	0.9	1.2	12.5	0.8	1.0	1.0	0.6	0.8	0.75
l_R (mkm)	8.5	16	5.0	7.0	10.4	3.7	5.2	9.0	1.7	1.5	4.0	1.3	1.7	3.0
d (mkm)	15	13	11	9.7	8	6.8	5.7	5	3.2	2.8	2.5	2	1.8	1.6
L/d	83	100	91	134	175	132	210	250	250	358	400	300	440	460
W	0.59	0.63	0.67	0.67	0.70	0.78	0.77	0.78	0.90	0.88	0.86	0.96	0.93	0.91
F_s (kcal/cm^{3}s)	35	23	120	90	76	380	278	180	2,235	2,340	950	5,140	3,790	2,150
F_0 (kcal/cm^{3}s)	14.5	–	–	35	–	–	70	–	–	170	–	–	330	–

Compatibility with polymers (DTA, calcd. values of activation energy and reaction order were used as indices for judging compatibility, HEM = RDX)[152]:

Polymer	*W* (% HEM)	Dec. peak (°C)	*n*	*E* (kcal mol^{-1})	ΔH_{dec} (kcal g^{-1})	ΔH_l (cal g^{-1})
-	100	240	0.8	80	0.49	30
PE	42	237	0.7	81	0.25	20
Epon 828 (anhydrous, cured)	42	220	1.9	107	0.54	–
Epon 828 (anhydrous, extracted)	43	–	–	–	–	8
Epon 828 (anhydrous, extracted)	42	224	1.7	105	–	6
PST	47	241	0.9	84	0.51	23
Epon 828 (BF_3 cured)	33	238	0.8	79	0.52	29
PAA	51	241	0.9	84	0.51	23
PMMA	47	239	1.1	66	0.58	–
PIBM	54	237	1.0	76	0.48	20
PEMA	38	238	1.3	70	0.66	–
Gantrez	55	219	–	–	–	–
PODA	53	238	0.6	76	0.48	22

Solubilty of RDX (g/100 g solvent) values from[164]:

Solvent	%	°C
Water	0.005	30
	0.025	50
	0.076	70
	0.19	90
	0.28	100
Alcohol	0.040	0
	0.105	20
	0.240	40
	0.579	60
	1.195	78
Acetone	7.3	20
	11.5	40
	18	60
Benzene	0.05	20
	0.09	40
	0.20	60
	0.41	80
Toluene	0.015	0
	0.02	20
	0.05	40
	0.13	60
	0.30	80
	0.65	100
Ethyl acetate	2.9	28
	18	94
CCl_4	0.005	50
	0.007	60
	0.009	70

MeOH	0.14	0
	0.23	20
	0.47	40
	1.1	60
Ether	0.05	10
	0.056	20
	0.076	30
TNT	4.4	80
	5.0	85
	5.55	90
	6.2	95
	7.0	100
	7.9	105
Isoamyl alcohol	0.02	0
	0.03	20
	0.065	40
	0.22	60
	0.54	80
	1.35	100
Methyl acetate	2.9	20
	3.3	30
	4.1	40
	5.6	50
β-Ethoxyethyl acetate	0.15	20
	0.16	30
	0.19	40
	0.25	50
Chlorobenzene	0.33	20
	0.44	30
	0.56	40
	0.74	50

Trichloroethylene	0.20	20
	0.22	30
	0.24	40
	0.26	50
Tetrachloroethane	0.09	38
Isopropanol	0.18	38
Isobutanol	0.0	23
$CHCl_3$	0.01	20
Mesityloxide	3.2	27
	12.2	97
Cyclohexanone	12.7	25
	25	97
Nitroethane	3.6	28
	19	93
Cyclopentanone	11.5	28
	37	90
Acetonitrile	11	28
	33	82
Methyl ethyl ketone	5.6	28
	14	95

RDX crystal structures[20, 21]:

	Hexogen[21, 42]	Hexogen[34]	α-RDX[49]	RDX-I (α-)[19, 38]	β-RDX[47]	β-RDX[47]	γ-RDX[51]	RDX[48]	RDX[48]	RDX[48]	RDX[20]
	Neutron diffraction		X-ray, single crystal		*	*	*Single crystal of α-RDX compressed to 0.1 GPa under hydrostatic conditions in a diamond anvil cell, pressure then increased to 5.20 GPa and data collected at this pressure				
Chemical formula	$C_3H_6N_6O_6$	$C_3H_6N_6O_6$	$C_3H_6N_6O_6$	$C_3H_6N_6O_6$	$C_3H_6N_6O_6$	$C_3H_6N_6O_6$	$C_3H_6N_6O_6$	$C_3H_6N_6O_6$	$C_3H_6N_6O_6$	$C_3H_6N_6O_6$	$C_3H_6N_6O_6$
Molecular weight [g mol^{-1}]	222.14	222.14	222.14	222.14	222.14	222.14	222.14	222.14	222.14	222.14	222.14
Crystal system	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic

Space group	*P b c a* (no. 61)		*P b c a* (no. 61)	*P b c a* (no. 61)	*P c a* 2_1 (no. 29)	*P c a* 2_1 (no. 29)	*P c a* 2_1 (no. 29)	*P b c a* (no. 61)	*P b c a* (no. 61)	*P b c a* (no. 61)	
a [Å]	13.182(2)	13.22	11.4195(8)	13.18	15.1267(11)	15.0972(7)	12.5650(19)	11.3790(2)	11.4425(3)	11.6103(4)	13.18
b [Å]	11.574(2)	11.61	10.5861(7)	11.57	7.4563(6)	7.5463(4)	9.4769(6)	10.5694(2)	10.6106(3)	10.7291(3)	11.57
c [Å]	10.709(2)	10.72	13.1401(9)	10.71	14.3719(11)	14.4316(6)	10.9297(9)	13.1314(2)	13.1558(4)	13.2013(4)	10.71
α [°]	90	90	90	90	90	90	90	90	90	90	90
β [°]	90	90	90	90	90	90	90	90	90	90	90
γ [°]	90	90	90	90	90	90	90	90	90	90	90
V [Å^3]			1588.48(19)	1633.2	1621.0(2)	1644.16(13)	1301.5(2)	1579.30	1597.27	1644.46	
Z	8		8	8	8	8	8	8	8	8	8
ρ_{calc} [g cm^{-3}]	1.806		1.858	1.80643	1.820	1.795	2.267	1.869	1.847	1.794	
T [K]			90		150	273	293	20	120	298	

* Diamond anvil cell investigations show that β- and γ- forms of RDX exist at high pressures. γ-RDX is stable >3.8 GPa between RT and 225 °C, but spontaneously reverts to α-RDX if the pressure is reduced to pressures of 3.5 GPa. β-RDX is stable >225 °C at pressures between 2.5–7 GPa. β-RDX reverts to α-RDX if the pressure is reduced to *ca.* 1 atmosphere.

Effects of temperature and pressure on the crystallization of RDX from cyclohexanone solution using supercritical CO_2 ($scCO_2$) as the antisolvent[133]:

Effect of pressure on the shape and size of RDX crystals @ 323 K[133]

Pressure (MPa)	Shape	Mean particle size (μm)	Pressure (MPa)	Shape	Mean particle size (μm)
9.8	Irregular	10.5	14.7	Granular	4.7
11.7	Irregular	11.9	15.7	Granular	5.2
12.7	Granular	6.5	17.6	Granular	4.5
13.7	Granular	5.1			

Effect of temperature on the shape and size of RDX crystals @ 13.7 MPa[133]

Temperature (K)	Shape	Mean particle size (μm)	Temperature (K)	Shape	Mean particle size (μm)
295	Plate-like	6.1	313	Granular	3.0
308	Irregular	8.7	323	Granular	2.9
311	Granular	2.9	353	Granular	2.9

Effect of flow rate ratio of $scCO_2$ to the solution on the shape and size of RDX crystals @ 13.7 MPa[133]

Soln. flow rate (mL/min)	$scCO_2$ flow rate (kg/h)	Flow rate ratio of $scCO_2$ to the soln.	Shape	Mean particle size (μm)
0.1	0.91 0.81	160 142	Granular Granular	2.6 2.9
0.3	0.85 0.75	50 44	Granular Granular	2.8 3.0
0.5	0.82	29	Irregular	4.2
1.0	0.81	14	Irregular	4.2–5.0
3.0	0.81	5	Irregular	7.5
10.0 10.0 10.0	0.81 0.35 0	1.4 0.6 0	Irregular Needle-like Needle-like	None None None

Solvent used and crystalline form obtained[164]:

Solvent	Crystalline form	Solvent	Crystalline form
Acetone	Hexagonal-thick	Methyl ethyl ketone	Coarse plates
Cyclohexanone	Cubic (massive form)	Nitroethane	Plates
Nitromethane	Plates	Isopropylacetate	Long prisms
Acetonitrile	Plates	Mesityloxide	Plates
1-Nitropropane	Short needles	*N*-Amylacetate	Prisms
2-Nitropropane	Short needles	Dimethylcarbonate	Plates
2,4-Pentanedione	Flat prisms	Diethylcarbonate	Prisms
Methylisobutylketone	Long prisms	Isoamylacetate	Prisms
N-Propylacetate	Long prisms, some cubic	Ethylpropionate	Fairly thick hexagonal plates
N-Butylformate	Long prisms	Methyl-*N*-butyrate	Needles
Ethyl Acetate	Hexagonal plates	Cyclopentanone	Hexagonal plates
N-Propylpropionate	Short prisms, some cubic	Acrylonitrile	Flat plates
Butylacetate	Long prisms	Methylcellosolveacetate	Massive hexagons and prisms

Monoclinic crystals obtained from recryst. from acetone[172], tetragonal crystals obtained from nitric acid[172]

Failure diameters of lead and booster explosives[174]:

Explosive	Confinement, in.		
	Fabric (detonating cord)	Aluminum (0.006 walls)	Lead (MDF)
RDX			<0.02
RDX/calcium stearate, 98/2	0.14–0.17	0.08–0.12	

Figure 10 data from[175]:

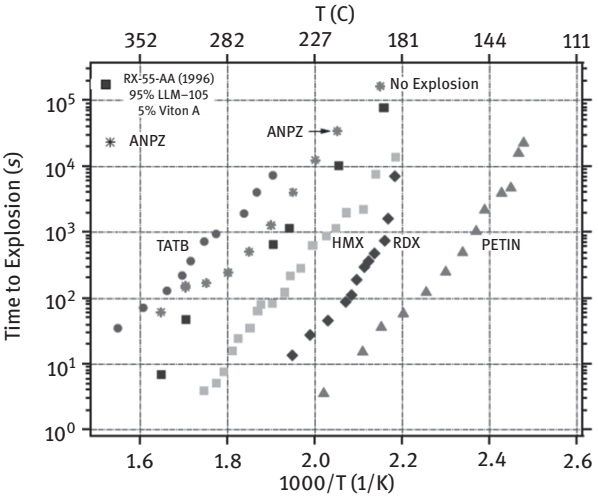

Fig. 10: ODTX results of ANPZ and TATB, HMX, RDX and PETN[175].

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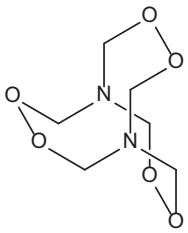
HMTD

Name [German, acronym]: 3,4,8,9,12,13-Hexaoxa-1,6-diaza-bicyclo-[4,4,4]-tetradecane, 1,6-diaza-3,4,8,9,12,13-hexaoxabicyclo[4.4.4] tetradecane, hexamethylenetriperoxidediamine [HMTD]

Main (potential) use: Improvised explosive, patented as primary explosive in detonators but no widespread use due to stability and compatibility issues[16], too reactive chemically and too unstable for practical use[19]

Structural formula:



	HMTD
Formula	$C_6H_{12}N_2O_6$
Molecular mass [g mol^{-1}]	208.17
Appearance at RT	Colorless crystals[16], white orthorhombic crystals[1]
IS [J]	2 (<100 µm), 0.06 kg/m[3], 0.015 kg/m[3], 0.6[5], 0.06 kg m (lit.)[7], 0.015 kg m (BAM, lowest impact energy for $^0/_6$ positive tests)[7], 3 cm (2 kg mass)[8, 19], impact sensitive when dry or wet[16], spontaneous explosion @ RT possible (no obvious external stimuli) for crystals obtained from $CHCl_3$[16], no spontaneous explosions reported for raw material[16]
FS [N]	<5 (<100 µm), 0.63[4], 0.1[5, 11], 0.01 (lit.)[7], <0.5 kgf (BAM, below detection limit of apparatus)[7]
ESD [J]	0.003 (<100 µm), 0.0088[5]
N [%]	13.46
$\Omega(CO_2)$ [%]	–92.2
$T_{m.p.}$ [°C]	Decomposes without melting (ignition temperature ~200 °C)[1], 152–153[10], 145[14, 21], 152–153 (dec. with explosion)[11], 144–145 (dec. with explosion)[11], 160–165 (dec. with explosion)[11]

$T_{dec.}$ [°C]	119 (DSC @ 5 °C/min), 170 (DSC @ 20 °C/min)[3], 150[5], 170 (exotherm peak, DSC @ 20 °C/min)[7], 125–140 (onset, DTA/TG)[1], 150 (onset)[11], 150 (onset), 161 (exo peak max) (DSC @ 20 K/min, crude HMTD, sealed microampules)[20]		
ρ [g cm^{-3}]	1.582 (@ 295 K), 1.597 (crystal)[5, 14, 16], 1.597 (crystal @ 150 K)[10], 1.575 (crystal @ 295 K)[9], 1.582 (crystal @ 21 °C)[8], 1.57 (lit.)[16], 1.57 (true density (20°/20°)[19], 0.66 (apparent ρ after being placed in tube and tapped)[19], 0.91 (ρ after being compressed in detonator capsule under pressure of 2,500 lb/in^2)[19] Loading ρ: 1.05 @ 100 atm.[14], 1.15 @ 200 atm[14], 1.30 @ 800 atm[14] 1.57 (crystal)[1], 0.66 (orthorhombic crystal bulk density)[1], fine crystals can be pressed up to 1.3 g cm^{-3}, but coarse crystals explode[1]		
Heat of formation	–1,731 kJ/kg ($\Delta_f H°$)[5], 385 cal/g[14], -363 kJ/mol (*Muraour*)[16], –335 kJ/mol (*Danilov*)[16], -360.2 kJ/mol (enthalpy of form., exptl.)[22], -350.1 kJ/mol (enthalpy of form., calcd., emp.)[22], -526.2 kJ/mol (enthalpy of form., calcd., S-D method)[22]		
Heat of combustion	4,295 cal/g (@ C^V, H_2O (liq.))[14]		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]	4,713	1,058 kJ/mol[16]	5,080[1, 5, 15]
T_{ex} [K]	2,841		
$p_{C\text{-}J}$ [kbar]	203		
VoD [m s^{-1}]	7,372	2,820 (@ 0.38 g cm^{-3})[16] 4,511 (@ 0.88 g cm^{-3})[16] 4,500 (@ 1.05 g cm^{-3})[16] 5,100 (@ 1.15 g cm^{-3})[16]	4,511 (@ 0.88 g cm^{-3}, 0.2 in diameter column)[14, 19] 2,820 (@ 0.38 g cm^{-3}, glass confinement)[15] 4,510 (@ 0.88 g cm^{-3})[1, 5, 6] 5,100 (@ 1.10 g cm^{-3})[1, 12, 14] 4,500 (@ 0.88 g cm^{-3})[5, 6] 16,700 ft/s (@ 1.1 g/mL)[21]
V_0 [L kg^{-1}]	823	813 dm^3 kg^{-1}[16]	1,075[2]

<table>
<tr><td>Trauzl test [cm^3, % TNT]</td><td>60% TNT[12], 60% TNT or 230% MF[14], 242 cm^3[16], 330 cm^3 (110% TNT)[16], 330 (10 g sample)[11]</td></tr>
<tr><td>Sand test [g]</td><td>0.5 g HMTD @ 1,000 psi crushes 42.5 g sand (cf. 16.5 g MF)[14], 71% TNT[16], pulverizes 2.5–3 times as much sand as mercury fulminate[19]</td></tr>
<tr><td>Initiating efficiency</td><td>0.05 g with reinforcing cap for tetryl[16], 0.06 g without reinforcing cap for tetryl[16], 0.08 g with reinforcing cap for TNT[16], 0.10 g without reinforcing cap for TNT[16], minimal charge in a No. 8 detonator towards tetryl = 0.05 g[1]

Minimum initiating efficiency of HMTD to detonate 0.4 of high explosive, HMTD compressed in detonator capsule under pressure of 1,000 lb/in^2[19]:

<table>
<tr><th rowspan="2">High explosive</th><th colspan="2">Minimum initiating charge (g) of HMTD</th></tr>
<tr><th>With reinforcing cap</th><th>Without reinforcing cap</th></tr>
<tr><td>TNT</td><td>0.08</td><td>0.10</td></tr>
<tr><td>PA</td><td>0.05</td><td>0.06</td></tr>
<tr><td>Tetryl</td><td>0.05</td><td>0.06</td></tr>
<tr><td>Ammonium picrate</td><td>0.30</td><td>0.30</td></tr>
<tr><td>Tetranitroaniline</td><td>0.05</td><td>0.05</td></tr>
<tr><td>Guanidinium picrate</td><td>0.13</td><td>0.15</td></tr>
<tr><td>Trinitroresorcinol</td><td>0.08</td><td>0.10</td></tr>
<tr><td>Hexanitrodiphenylamine</td><td>0.05</td><td>0.05</td></tr>
<tr><td>Trinitrobenzaldehyde</td><td>0.08</td><td>0.10</td></tr>
</table>
</td></tr>
<tr><td>Dead pressing</td><td>Not dead-pressed @ 76 MPa[16], not dead-pressed @ 294 MPa[16], explosions occur on pressing coarse crystals ≥20 MPa[16], not dead-pressed by pressure of 11,000 lb/in^2[19]</td></tr>
<tr><td>5 s explosion T [°C]
Explosion T [°C]

5 s ignition T [°C]
3 s ignition T [°C]

Ignition T [°C]</td><td>
explodes instantly @ 200[14, 16], explodes @ 130 when gradually heated[14], small quantity decomposes without exploding when dropped onto molten metal @ 190 °C but instantly detonated if dropped onto 200 °C[19]
<149[13]
149 (0.05 g sample)[16, 19], ignites after 3 s @ 149 on being thrown onto heated metal surface[14]
200 (dropping on preheated Wood's alloy)[14], 125–400 range[16], 139 (@ 20 °C/min)[16], 200 (instantly)[21], ~200 (1 s)[1]</td></tr>
</table>

<table>
<tr><td>Thermal stability</td><td>stable for considerable time if stored in air or in airtight containers[1], stable if maintained under layer of water @ RT for ~4 weeks[1], complete dec. after storage under water for 4 months[1]

Thermal stability in storage: 70% weight loss in 300 days @ 50 °C, 150 days @ 70 °C and 5–20 days @ 90 °C[14]

Thermal stability at different temperatures[19]:

<table>
<tr><td>% weight loss</td><td>60 °C</td><td>75 °C</td><td>100 °C</td></tr>
<tr><td>2 h</td><td>0.10</td><td>0.25</td><td>–</td></tr>
<tr><td>8 h</td><td>0.35</td><td>0.60</td><td>29.60</td></tr>
<tr><td>24 h</td><td>0.50</td><td>1.30</td><td>67.95</td></tr>
<tr><td>48 h</td><td>0.50</td><td>2.25</td><td>-</td></tr>
</table>

Slight hydrolysis occurs in cold H_2O after several months[16], stable if stored under H_2O for 4 weeks @ 30 °C[16], slow dec. @ 40 °C[16]</td></tr>
<tr><td>Activation energy for dec. [kJ/mol]</td><td>–120[17]</td></tr>
<tr><td>Vapor pressure [atm @ °C]</td><td>5.3×10^{-6} Pa @ 20 °C (extrapolated form exptl. data)[17]</td></tr>
<tr><td>Enthalpy of sublimation [kJ/mol]</td><td>–93.5 ± 3 (based on exptl. values)[17]</td></tr>
<tr><td>Solubility [g/mL]</td><td>Essentially insoluble in water and organic solvents[1]

Solubility in solvents @ 22 °C[16]:

<table>
<tr><td>Solvent</td><td>Solubility (g/100 g solvent)</td></tr>
<tr><td>EtOH</td><td>< 0.01</td></tr>
<tr><td>Acetone</td><td>0.33</td></tr>
<tr><td>CS_2</td><td>< 0.01</td></tr>
<tr><td>CCl_4</td><td>0.013</td></tr>
<tr><td>$CHCl_3$</td><td>0.64</td></tr>
<tr><td>Et_2O</td><td>0.017</td></tr>
<tr><td>Ethyl-1,2-diyl diacetate</td><td>0.90</td></tr>
<tr><td>Glacial acetic acid</td><td>0.14</td></tr>
<tr><td>H_2O</td><td>0.01</td></tr>
</table>
</td></tr>
</table>

<table>
<tr><td></td><td>Slightly soluble in CH_3CN, DMSO, DMF, $CHCl_3$[16], almost insoluble in H_2O and common organic solvents @ RT[19], only limited solubility in even more polar solvents[20], large volumes of ethyl acetate and acetone required for recryst.[20]</td></tr>
<tr><td>Hygroscopicity</td><td>Slightly hygroscopic[16], negligible hygroscopicity[1]</td></tr>
<tr><td>Compatibility</td><td>Slow dec. >40 °C in presence of moisture[1], hydrolysis by acids and bases @ RT[1], doesn't react with aqueous solns. of $NaHNO_3$, Na_2CO_3 or NH_3[1], slow dec. by traces of acids and metal ions[1], readily reduced by Zn/HCl[1], readily reduced by aqueous and alcoholic solns. of $SnCl_2$[1], readily reduced by HBr or HI solns.[1], dry HMTD doesn't react with metals but in the presence of moisture facile corrosion of metals occurs[1]

Effect of solid additives on stability (HMTD maintained @ 60 °C for 7 days @ 30% rel. humidity, no H_2O added)[18]:

<table>
<tr><th>HMTD solid additive (15%)</th><th>Average HMTD remaining (%)</th></tr>
<tr><td>None</td><td>87</td></tr>
<tr><td>$NaHCO_3$</td><td>87</td></tr>
<tr><td>KH_2PO_4</td><td>96</td></tr>
<tr><td>NaOH</td><td>75</td></tr>
<tr><td>KO^tBu</td><td>80</td></tr>
<tr><td>Citric acid</td><td>13</td></tr>
</table>

HMTD dec. by conc. mineral acid[18], rapid dec. with aq. basic solns.[18], after 2 weeks storage @ high humidity complete dec.[18]

% HMTD remaining after storage @ 60 °C for various lengths of time under various rel. humidities[18]:

<table>
<tr><th>Rel. humidity (%)</th><th>1 week</th><th>2 weeks</th><th>4 weeks</th></tr>
<tr><td>0</td><td>100</td><td>85</td><td>60</td></tr>
<tr><td>30</td><td>90</td><td>85</td><td>25</td></tr>
<tr><td>75</td><td>35</td><td>0</td><td>0</td></tr>
<tr><td>100</td><td>1</td><td>0</td><td>0</td></tr>
</table>
</td></tr>
</table>

Effect of humidity on crude HMTD stored @ 60 °C[18]:

Time (days)	Dry	75% rel. humidity
0	100	–
1	100	~ 95
2	–	~ 98
3	~ 98	~ 82
4	–	~ 65
5	–	~ 55
6	–	~ 52
7	~ 95	~ 45

Effect of humidity on recrystallized HMTD stored @ 60 °C[18]:

Time (days)	Dry	75% rel. humidity
0	100	–
4	100	~ 85
6	–	~ 80
8	–	~ 60
10	–	~ 45
11	~ 91	–
12	–	20
15	~ 90	–

Destabilized by H_2O and citric acid[20]

Effect of solid additives on HTMD stability, 30% rel. humidity, 15% solid additive, 60 °C, 1 week[20]:

Solid additive	Average % HTMD remaining	Solid additive	Average % HTMD remaining
None	87	NaOH	75
$NaHCO_3$	87	K^tBuO	80
KH_2PO_4	96	Citric acid	13

Effect of humidity on HTMD, % HTMD remaining after HTMD maintained @ 60 °C @ different relative humidity[20]:

% rel. humidity	1 week	2 weeks	4 weeks
0	100	82	58
30	90	85	30
75	35	HTMD completely degraded	
100	5	HTMD completely degraded	

Effect of humidity on crude HTMD, % crude HTMD remaining after being maintained @ 60 °C with 75% relative humidity or dry[20]:

Time (days)	Dry conditions	75% rel. humidity
0	100	–
1	100	94
2	–	97
3	97	85
4	–	65
5	–	55
6	–	54
7	95	45

Effect of humidity on recryst. HTMD, % recryst. HTMD remaining after being maintained @ 60 °C with 75% relative humidity or dry[20]:

Time (days)	Dry conditions	75% rel. humidity
0	100	–
4	100	85
6		80
8		65
10		40
11	95	–
12		20
15	92	

Effect of additives on $T_{dec.}$ of crude HMTD (DSC @ 20 K/min, sealed micro ampules)[20]:

Sample	$T_{exo\ onset}$ (°C)	$T_{exo\ peak\ max}$ (°C)	Heat released (J/g)
HMTD crude	159	161	2,100
HMTD rec 70/30 EA/CAN	168	171	3,200
crude HMTD + aqueous solution			
HMTD + 2 µl H_2O	136	140	3,100
HMTD rec 70/30 EA/ACN + 2 ul H_2O	140	143	3,200
HMTD + 2 µl pH 4 buffer	126	129	3,700
HMTD + 2 µl pH 7 buffer	134	137	3,300
HMTD + 2 µl pH 10 buffer	137	139	3,100
crude HMTD + solvents			
HMTD + 2 µl ACN	152	178	3,000
HMTD + 2 µl benzene	166	172	3,200
HMTD + 2 µl EtOH	153	164	2,800
HMTD + 2 µl EtAc	156	169	2,800
crude HMTD + solid acids			
HMTD + 15% H_2PO_4	163	165	2,100
HMTD + 15% KH phthalate	156	157	1900
HMTD 15% benzoic acid	155	160	2,600
HMTD + 15% ascorbic acid	146	148	2,000
HMTD + 15% citric acid	134	137	2,800
HMTD + 15% sulfanilic acid	122	125	2,400
HMTD + 15% O phthalic acid	143	145	2,000
crude HMTD + solid bases			
HMTD + 15% melamine	158	159	2,000
HMTD + 15% $NaHCO_3$	163	164	1,300
HMTD + 15% KH_2PO_4	163	165	2,100
HMTD + 15% NaOH	160	161	2,300
HMTD + 30% NaOH	162	164	2,100
HMTD + 15% K tertbutoxide	159	160	2,200

	Loss of power on exposure to moisture, but power returns to maximum after drying[21]
Dipole moment [Debye]	0.68 (from quantum chemical calcs.)[17]
ΔH°_{sub} [kcal/mol]	15.6[11]
Laser sensitivity	Threshold of initiation with beam of Q-switch neodymium glass laser (λ = 1.06 μm, τ = 30 ns) = ~ 40 mJ/cm^2[1]

Brisance: could not be evaluated due to HMTD's high sensitivity. HMTD could not be pressed and underwent spontaneous explosion during sample preparation[7].

	HMTD[8]	**HMTD**[9]	**HMTD**[10]
Chemical formula	$C_6H_{12}N_2O_6$	$C_6H_{12}N_2O_6$	$C_6H_{12}N_2O_6$
Molecular weight [g mol^{-1}]	208.17	208.17	208.17
Crystal system	Rhombohedral	Rhombohedral	Rhombohedral
Space group	*R* 3 *m* (no. 160)	*R* 3 (no. 146)	*R* 3 *m* (no. 160)
a [Å]	10.417(5)	6.4603(2)	10.3982(4)
b [Å]	10.417(5)	6.4603(2)	10.3982(4)
c [Å]	6.975(3)	6.4603(2)	6.9332(4)
α [°]	90	107.80(3)	90
β [°]	90	107.80(3)	90
γ [°]	120	107.80(3)	120
V [Å^3]	655.481	219.461	649.203
Z	3	1	3
ρ_{calc} [g cm^{-3}]	1.582	1.575	1.597
T [K]	21 °C	295	150

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Hydrazine

Name [German, acronym]: Hydrazine [hydrazin]
Main (potential) use: Propellants for flight control rockets[1], component of hypergolic systems[8], fuel for some high-performance rockets[14]

Structural formula:

	Hydrazine
Formula	H_4N_2
Molecular mass [g mol^{-1}]	32.05 (50.06 hydrate)
Appearance at room temperature	Colorless liquid with ammonia odor[10], hydrate is a fuming colorless liquid[10], clear fuming liquid[13], colorless, fuming hygroscopic liquid with fishy odor[14], colorless, oily liquid that fumes in air[15], fuming, refractive liquid with faint odor (hydrazine hydrate)[15]
FS [N]	Completely insensitive[7]
ESD [J]	Completely insensitive[7]
N [%]	87.42 (55.95 hydrate)
$\Omega(CO_2)$ [%]	−99.8
$T_{m.p.}$ [°C]	2.01[1], 2.0[2, 4, 15], 1.54[8], 1.3 (freezing point)[10], 1.4 (freezing point)[11], −40 (freezing point of hydrate)[10], 2 (freezing point)[13], 2[14], −517 (hydrazine hydrate)[15], 2.0 (freezing point)[16]
$T_{b.p.}$ [°C]	113.5[8, 10, 13], 118.5 (hydrate)[10], 113[11], 114[14], bp_{760} = 113.5[15], bp_{71} = 56[15], $bp_{5\ atm.}$ = 170[15], $bp_{10\ atm.}$ = 200[15], $bpt_{20\ atm.}$ = 236[15], bp_{760} = 118–119 (hydrazine hydrate)[15], bp_{26} = 47 (hydrazine hydrate)[15]
$T_{dec.}$ [°C]	199.85[3]
ρ [g cm^{-3}]	1.004[1, 8], 1.0065 (@ 295.45 K)[4], 1.008[5], sp. gr. = 1.004 (@ 25°/4°)[7], 1.008 (@ 20 °C)[11], 1.011 (@ TMD, liq. with 0.7% H_2O)[12], 1.00[14, 16], $d^{-5}{}_4$ = 1.146[15], $d^0{}_4$ = 1.0253[15], $d^2{}_4$ = 1.024[15], $d^{15}{}_4$ = 1.011[15], $d^{25}{}_4$ = 1.0036[15], $d^{35}{}_4$ = 0.9955[15], 1 gallon of commercial hydrazine weighs 8.38 lbs[15], $n^{22.3}{}_D$ = 1.46979[15], $n^{35}{}_D$ = 1.46444[15], d^{21} = 1.03 (hydrazine hydrate)[15], $n^{20}{}_D$ = 1.42842 (hydrazine hydrate)[15]
Heat of formation	1,580 kJ/kg (enthalpy of form.)[1], 376 cal/g[5], 12.05 kcal/mol (@ 298.15 K)[11], 50.63 kJ/mol (enthalpy of form.)[8, 14], 46.23 kJ/mol (heat of form., with 0.7% H_2O)[12]

Heat of combustion	148.635 kcal/mol (liq.)[7]	
	Calcd. (EXPLO5 6.03)	Exptl.
$-\Delta_{ex}U^{o}$ [kJ kg^{-1}]	3,388	
T_{ex} [K]	1,864	
$p_{C\text{-}J}$ [GPa]	13.2	
VoD [m s^{-1}]	7,700	
V_0 [L kg^{-1}]	1,347	
I_s [s]	294.0[16], I_d = 444.0[16]	

Critical temperature [°C]	380[11, 15]
Critical pressure [atm]	145[11], 14 atm.[15]
Initiating efficiency	liquid cannot be detonated by No. 8 blasting cap[10], vapors sparked @ 1000 °C will explode[10]
5 s explosion T [°C] Detonating T [°C]	 232[10]
Thermal stability	Stable under the extremes of heat and cold experienced on long-term storage[11], freezing does not affect its chemical properties[11], in the presence of catalysts such as Cu, Mo or iron oxide dec. may occur @ RT[11], explodes during distillation if traces of air are present[15], can be stored for years if sealed in glass and stored in a cool, dark place[15]
Vapor pressure [atm. @ °C]	1.9 kPa @ 25 °C[8], 0.204 psi @ 20 °C[11], 2.806 psi @ 70 °C[11]
Viscosity [cp]	0.9736 @ 20 °C[11]
Burn rate [mm/s]	Burns with violet flame[15]
Solubility [g/mL]	Extremely soluble in water[10], soluble in EtOH[10], very soluble in water[14], miscible with water, MeOH, EtOH, PrOH, ^{i}ButOH[15], forms azeotropic mixture with water[15], hydrazine hydrate = miscible with water and EtOH, but insoluble in $CHCl_3$ and Et_2O[15]
Hygrosopicity	Hygroscopic[13, 14]
Photosensitivity	Affected by UV[15]
Compatibility	Attacks rubber, cork, mild steel, some common metals[10], generally stored in stainless steel tanks and drums, or PVC-lined or coated drums[10], glass, iron or aluminum containers are not used for the hydrate[10], in the presence of catalysts such as Cu, Mo or iron oxide dec. may occur @ RT[11], compatible with stainless steel (303, 304, 316, service limited to 160°F, 321 and 347), Ni Al (3003, 5052, 5154, 1060 and 6061), Teflon, high-density polyethylene and unplasticized Kel-F[11], some compatibility with Q-Seal lubricant[11],

	thermodynamically unstable and readily decomposes on some metal surfaces *e.g.* rough stainless steel[13], fumes in air[15], hydrazine hydrate = very strong base, very corrosive, attacks glass, rubber, cork ut not stainless steel, V_2A steel, Allegheny stainless 304 and 347[15], Mo steels such as Alleghany stainless 316 should not be used for hydrazine hydrate[15]
Decomposition activation energy [kJ/mol]	38.3 (gold pan, Kissinger method)[9], 140.5 (glass capillary, Kissinger method)[9], 41.0 (gold pan, Ozawa method)[9], 140.7 (glass capillary, Ozawa method)[9]
Heat of vaporization [kcal/mol]	10.7 @ 25.0 °C[11]
Heat of fusion [kcal/mol]	3.025 (latent heat of fusion (mp))[15]
Specific heat [cal/g]	0.738 @ 25 °C[11]
Flash point [°C]	38[14], 52 (flash and fire point)[15]
Autoignition *T* [°C]	270[14]
Dipole moment	1.83–1.90[15]
Dielectric constant	51.7 (25°)[15]
K_1	~9 × 10^{-7} (@ 25°)[15]

	Hydrazine[6]
Chemical formula	H_4N_2
Molecular weight [g mol^{-1}]	32.05
Crystal system	Monoclinic
Space group	*P* 2_1/ *m* (no. 11)
a [Å]	3.56
b [Å]	5.78
c [Å]	4.53
α [°]	90
β [°]	109.5
γ [°]	90
V [$Å^3$]	
Z	2
ρ_{calc} [g cm^{-3}]	
T [K]	

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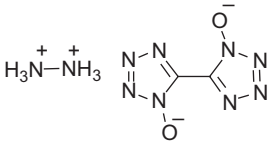
Hydrazine 5,5′-bitetrazole-1,1′-diolate

Name [German, acronym]: Hydrazine 5,5′-bitetrazole-1,1′-diolate [HA.BTO]
Main (potential) use: Secondary explosive
Structural formula:



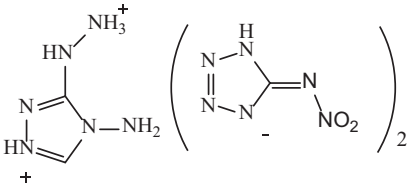
	HA.BTO	
Formula	$C_2H_6N_{10}O_2$ $[N_2H_6]^{2+}[C_2N_8O_2]^{2-}$	
Molecular mass [g mol^{-1}]	202.17	
Appearance at RT		
IS [J]	28	
FS [N]	120	
N [%]	69.3	
$\Omega(CO_2)$ [%]	−39.5	
$T_{m.p.}$ [°C]		
$T_{dec.}$ [°C]	207	
ρ [g cm^{-3}]	1.923 (@ 153 K), 1.913 (@ 298 K)	
Heat of formation	425.6 kJ/mol ($\Delta_f H°$)	
	Calcd. (K-J)	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]		
T_{ex} [K]		
$p_{C\text{-}J}$ [kbar]	361	278[10]
VoD [m s^{-1}]	8931 (@ TMD)	
V_0 [L kg^{-1}]		

3-Hydrazinium-4-amino-1*H*-1,2,4-triazolium di(5-nitramino-tetrazolate)

Name [German, acronym]: 3-Hydrazinium-4-amino-1*H*-1,2,4-triazolium di(5-nitramino-tetrazolate), [HATr.2NATZ]

Main (potential) use: Secondary explosive

Structural formula:



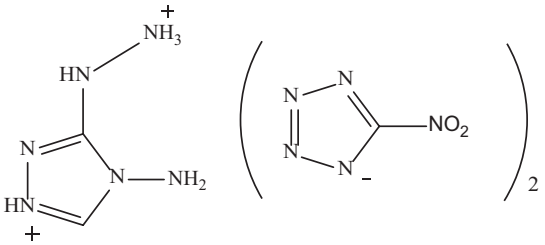
	HATr.2NATZ	
Formula	$C_4H_{10}N_{18}O_4$, $[C_2H_8N_6]^{2+}[CHN_6O_2]^{-}{}_2$	
Molecular mass [g mol^{-1}]	374.11	
Appearance at RT		
IS [J]	4	
N [%]	67.3	
$\Omega(CO_2)$ [%]	−38.49	
$T_{dec.}$ [°C]	211	
ρ [g cm^{-3}]	1.755 (contains crystal water), 1.795 (@ 298 K)	
Heat of formation	176.1 kJ/mol ($\Delta H_f°$)	
	Calcd. (K-J)	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]		
T_{ex} [K]		
$p_{C\text{-}J}$ [kbar]	286	
VoD [m s^{-1}]	8039 (@ TMD)	
V_0 [L kg^{-1}]		

3-Hydrazinium-4-amino-1*H*-1,2,4-triazolium di(5-nitro-tetrazolate)

Name [German, acronym]: 3-Hydrazinium-4-amino-1*H*-1,2,4-triazolium di(5-nitrotetrazolate) [HATr.2NTZ]

Main (potential) use: Secondary explosive

Structural formula:



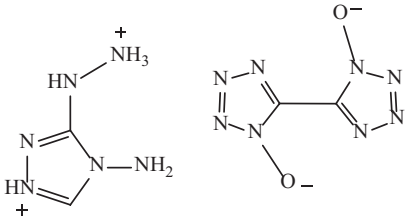
	HATr.2NTZ	
Formula	$C_4H_8N_{16}O_4$, $[C_2H_8N_6]^{2+}[CN_5O_2]_2^-$	
Molecular mass [g mol^{-1}]	344.09	
Appearance at RT		
IS [J]	4	
N [%]	65.11	
Ω(CO_2) [%]	−37.20	
$T_{dec.}$ [°C]	188	
ρ [g cm^{-3}]	1.711 (@ 298 K)	
Heat of formation	507.0 kJ/mol ($\Delta H_f°$)	
	Calcd. (K-J)	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]		
T_{ex} [K]		
$p_{C\text{-}J}$ [kbar]	253	
VoD [m s^{-1}]	7,665 (@ TMD)	
V_0 [L kg^{-1}]		

3-Hydrazinium-4-amino-1*H*-1,2,4-triazolium 1*H*,1′*H*-5,5′-bitetrazole-1,1′-diolate

Name [German, acronym]: 3-Hydrazinium-4-amino-1*H*-1,2,4-triazolium 1*H*,1′*H*-5,5′-bitetrazole-1,1′-diolate [HATr.BTO]

Main (potential) use: Secondary explosive

Structural formula:



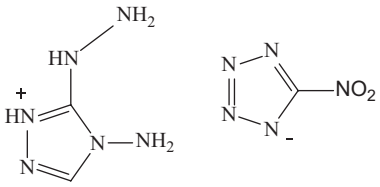
	HATr.BTO	
Formula	$C_4H_8N_{14}O_2$, $[C_2H_8N_6]^{2+}[C_2N_8O_2]^{2-}$	
Molecular mass [g mol^{-1}]	284.20	
Appearance at RT		
IS [J]	18	
N [%]	69.0	
Ω(CO_2) [%]	−56.30	
$T_{dec.}$ [°C]	249	
ρ [g cm^{-3}]	1.722 (@ 298 K)	
Heat of formation	587.7 kJ/mol ($\Delta H_f°$)	
	Calcd. (K-J)	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]		
T_{ex} [K]		
$p_{C\text{-}J}$ [kbar]	224	
VoD [m s^{-1}]	7,206 (@ TMD)	
V_0 [L kg^{-1}]		

3-Hydrazinium-4-amino-1*H*-1,2,4-triazolium Nitrotetrazolate

Name [German, acronym]: 3-Hydrazinium-4-amino-1*H*-1,2,4-triazolium nitrotetrazolate [HATr.NTZ]

Main (potential) use: Secondary explosive

Structural formula:



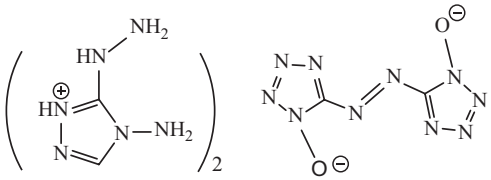
	HATr.NTZ	
Formula	$C_3H_7N_{11}O_2$, $[C_2H_7N_6]^+[CN_5O_2]^-$	
Molecular mass [g mol^{-1}]	284.20	
Appearance at RT		
IS [J]	8	
N [%]	61.4	
$\Omega(CO_2)$ [%]	−42.22	
$T_{dec.}$ [°C]	249	
ρ [g cm^{-3}]	1.657 (@ 298 K)	
Heat of formation	366.8 kJ/mol ($\Delta H_f°$)	
	Calcd. (K-J)	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]		
T_{ex} [K]		
$p_{C\text{-}J}$ [kbar]	194	
VoD [m s^{-1}]	6,720	
V_0 [L kg^{-1}]		

3-Hydrazino-4-amino-2*H*-1,2,4-triazolium 1*H*,1′*H*-5,5′-azotetrazole-1,1′-diolate

Name [German, acronym]: 3-Hydrazino-4-amino-2*H*-1,2,4-triazolium 1*H*,1′*H*-5,5′-azotetrazole-1,1′-diolate [2HATr.DHazo]

Main (potential) use: Secondary explosive

Structural formula:



	2HATr.DHazo	
Formula	$C_6H_{14}N_{22}O_2$, $[C_2H_7N_6]_2^+[C_2N_{10}O_2]^{2-}$	
Molecular mass [g mol^{-1}]	426.17	
Appearance at RT		
IS [J]	25	
N [%]	72.28	
$\Omega(CO_2)$ [%]	−63.82	
$T_{dec.}$ [°C]	183	
ρ [g cm^{-3}]	1.683 (@ 298 K)	
Heat of formation	768.7 kJ/mol ($\Delta H_f°$)	
	Calcd. (K-J)	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]		
T_{ex} [K]		
$p_{C\text{-}J}$ [kbar]	244	
VoD [m s^{-1}]	7,577 (@ TMD)	
V_0 [L kg^{-1}]		

Hydrazinium azide

Name [German, acronym]: Hydrazine azide, [Hydrazinium azid]
Main (potential) use: Has found use in rocket fuel technology[1]
Structural formula:

	Hydrazinium azide		
Formula	H_5N_5		
Molecular mass [g mol^{-1}]	75.09		
Appearance at RT	white solid		
IS [J]	Not sensitive[1]		
FS [N]			
ESD [J]			
N [%]	93.3		
Ω(CO_2) [%]	−8.54		
$T_{m.p.}$ [°C]	~70.5[1]		
$T_{dec.}$ [°C]	~90[1]		
ρ [g cm^{-3}]	1.407 (X-ray)[2]		
Heat of formation			
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]			
T_{ex} [K]			
$p_{C\text{-}J}$ [kbar]			
VoD [m s^{-1}]			
V_0 [L kg^{-1}]			
Thermal stability	Explodes on heat shock[1]		
Solubility [g/mL]	190 g/100 mL H_2O @ 23 °C[1], solubility: 6% in MeOH, 1% in EtOH[1], insoluble in Et_2O[1]		
Hygroscopicity	Very hygroscopic[1]		
Flame test	Burns in flame with explosion[1]		

	Hydrazinium azide[2]
Chemical formula	N_5H_5
Molecular weight [g mol^{-1}]	75.07
Crystal system	Monoclinic
Space group	$P2_1/b$
a [Å]	5.663(2)
b [Å]	12.436(3)
c [Å]	5.506(2)
α [°]	90
β [°]	114.0 (0.1)
γ [°]	90
V [Å^3]	354.17
Z	4
ρ_{calc} [g cm^{-3}]	1.407
T [K]	

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Hydrazinium nitrate

Name [German, acronym]: Hydrazine nitrate, hydrazine mononitrate [hydrazinnitrat, HN, HzN]

Main (potential) use: Due to its low mpt. it can be used to prepare fusible mixtures with AN[18]

Structural formula:

$$N_2H_5^+\ NO_3^-$$

	Hydrazinium nitrate
Formula	$H_5N_3O_3$
Molecular mass [g mol^{-1}]	95.06
Appearance at RT	Exists in two crystalline forms: (i) stable form and (ii) labile form[18]
IS [J]	7.4[1], 50% probability @ 175 kg/cm (Bruceton method)[9], 32 kg/cm (ERL, type 12 tool)[9], 50 kg/cm (ERL, type 12 tool)[9], similar to that of tetryl[18]
FS [N]	similar to that of HMX[18]
N [%]	44.21
Ω(CO_2) [%]	8.4
$T_{phase\ transition}$ [°C]	β- converts to α-form @ room temp. ($\Delta H_{transition}$ = 2.0 kcal/mol)[9], exists in two crystalline forms: (i) stable form and (ii) labile form[18]
$T_{m.p.}$ [°C]	70.5[2], 62 (β-form)[9], 70 (α-form)[9], 70.7 (stable crystalline form)[18], 62.1 (labile crystalline form)[18]
$T_{dec.}$ [°C]	229[1], dec. begins @ 180, rapidly increases above 240 and becomes explosive @ 270[9]
ρ [g cm^{-3}]	1.64[1], 1.549 (@ 348.15 K)[2], 1.661[9], 1.685 (@ TMD, liq.)[21], 1.64 (compressed under pressure of 3,000 kg/cm^2)[18] ρ at different pressures[9]:

ρ (g cm^{-3})	pressure (kg/sq cm)
1.08	34
1.18	88
1.28	136
1.43	204
1.49	306
1.58	425
1.616	680
1.635	1020
1.64	1700

Heat of formation	−2,590.68 ± 10.12[3], −2,597 kJ/kg (enthalpy of form.)[1], −60.5 kcal/mol (ΔH_f)[9], 56.7 kcal/kg (ΔH_f°, @ C^v)[9], 59.8 kcal/kg (ΔH_f°, @ C^p)[9], −56.86 kcal/mol (ΔH_f°, exptl.)[17], −55.30 kcal/mol (ΔH_f°, exptl.)[17], -58.86 kcal/mol (ΔH_f°, exptl.)[19], −87.37 kcal/mol (ΔH_f°, calcd.)[19], −58.86 ± 0.23 kcal/mol (ΔH_f°, exptl.)[20], −246.9 kJ/mol[21], −247.0 kJ/mol (enthalpy of form., exptl.)[23], −300.2 kJ/mol (enthalpy of form., calcd., emp.)[23], −240.4 kJ/mol (enthalpy of form., calcd., S-D method)[23]		
Heat of combustion	112.1 kcal/kg (ΔH_c @ C^V)[9], 111.1 kcal/kg (ΔH_c @ C^P)[9]		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]	3,875	4,841 (calcd. K-J)[4] 891 cal/g[15] 3.87 MJ/kg (heat of explosion)[22]	4,979.8 ± 5.4[3] 4,827 [H_2O (l)][1] 3,735 [H_2O (g)][1]
T_{ex} [K]	2,682	1,218 (@ 1.68 g cm^{-3}, calcd.)[13]	
$p_{C\text{-}J}$ [GPa]	267	136 (calcd. K-J)[5] 290 (@ 1.68 g cm^{-3}, calcd.)[13] 319 (@ 1.626 g cm^{-3}, calcd., *Xiong*)[15]	
VoD [m s^{-1}]	8,583 (@ 1.64 g cm^{-3}, $\Delta_f H = -246.3$ kJ mol^{-1})	8,460 (@ 1.68 g cm^{-3})[13] 8,400 (@ 1.64 g cm^{-3} (TMD), calcd. R-P method)[14] 8,980 (@ 1.64 g cm^{-3} (TMD), calcd. *Aizenshtadt*)[14]	8,500 (@ 1.6 g cm^{-3}, pressed, 2 ½ in diameter cartridge, rotating mirror camera)[9] 5,640 (@ 1.25 g cm^{-3} (max. value), 30 mm diameter cartridge, 170 mm long)[9] 8,510 (@ 1.59 g cm^{-3}, 6.3 cm diameter charge of pressed HzN)[9] 8,690 (@ 1.60 g cm^{-3})[1] 8,500 (@ 75 °C (molten HzN), thin-film expts.)[9]

		8,500 (@ 1.64 g cm^{-3} (TMD), calcd., K-J)[14] 8,685 (@ 1.626 g cm^{-3}, calcd. *Xiong*)[15]	5,200 (@ 1.6 g cm^{-3}, pressed HzN, 1 in diameter cartridge, rotating mirror camera)[9] 5,600 (@ 1.6 g cm^{-3}, pressed HzN, $1^5/_8$ in diameter cartridge)[9] 7,980 (@ 1.63 g cm^{-3})[10] 8,360 (@ 1.63 g cm^{-3})[10] 8,691 (@ 1.626 g cm^{-3})[6, 15] 8,690 (@ 1.626 g cm^{-3})[7] HzN is readily detonated by an initiating cap, VoD of cartridge, 30 mm diameter placed in cardboard paper case[18]:

ρ (g/cm^3)	VoD (m/s)
1.00	3,900
1.20	5,200
1.25	5,640
1.30	5,440
1.45	5,000
1.57	3,250

V_0 [L kg^{-1}]	1,093		1,001[1, 8]

	HN[11]*	**HN**[12]*
Chemical formula	$H_5N_3O_3$	$H_5N_3O_3$
Molecular weight [g mol^{-1}]	95.06	95.06
Crystal system	Monoclinic	Monoclinic
Space group	$P\,2_1/\,n$ (no. 14)	$P\,2_1/\,n$ (no. 14)
a [Å]	7.9649(4)	8.015
b [Å]	5.6569(3)	5.725
c [Å]	8.1221(3)	8.156

α [°]	90	90
β [°]	91.340(3)	92.3
γ [°]	90	90
V [Å^3]	365.85	373.94
Z		
ρ_{calc} [g cm^{-3}]		
T [K]		

* Two polymorphs are known: α-HN (stable) and β-HN (unstable)[9]

Critical diameter [cm]	Increases with increasing water content[9]
Trauzl test	120.4 ± 0.5 (cf. PA = 100)[9]
Brisance	82 (cf. TNT = 100)[9]
Gap test	Card gap sensitivity = 6.25 cm[9]
Burn rate [mm/s]	Supports combustion in the open air but flame was extinguished on removal of ignition source[9], addition of 10 wt. % $K_2Cr_2O_7$ necessary to achieve stable burning[9]
Initiation sensitivity	Non-compressed HN with 0.5% moisture content detonated with cap containing 0.25 g MF[9], compressed to ρ = 1.60 g cm^{-3} required 1.5 g MF for detonation[9]
Flame T [°C]	2400 (equilibrium value of detonations)[9]
Compatibility	Ignites with permanganate, chromate or peroxides[9], ignites with metallic Zn, Cu or their oxides, sulfides, nitrides or carbides at slightly above HN mpt.[9]

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[22] N. Kubota, *Propellants and Explosives – Thermochemical Aspects of Combustion*, Wiley-VCH, **2002**.
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Hydrazinium nitroformate

Name [German, acronym]: Hydrazinium nitroformate [HNF]*
Main (potential) use: Possible new clean-burning, high-energy oxidizer for solid rocket propellants; possible oxidizer in high burn rate, high I_{sp} and thixotropic propellants[7], possible energetic oxidizer in high-performance, Cl-free solid propellant formulations[10], HNF-based propellants suggested as possible new storable composite propellants[10, 14], proposed as oxidizer in solid propellants since early 1970s[11], possible likely substitute for AP[17]

Structural formula:

$$N_2H_2^+ \; C(NO_2)_3^-$$

* There are four commercial grades of HNF: HNF-S, HNF-C, HNF-E and HNF-P (see table at end of section for details)[14]

	HNF
Formula	$CH_5N_5O_6$
Molecular mass [g mol^{-1}]	183.08
Appearance at RT	Yellow, needle-shaped solid on recryst. from MeOH/CTC [17, 18], yellow rods (HNF-P)[19], yellow needles (HNF-E)[19], yellow facetted dry rods (HNF-C)[19], diamond-shaped rods (HNF-S)[19]
IS [J]	4[1], $H_{50\%}$ = 10 cm (2.5 kg mass)[3], 15[4], 1.6 (BAM, Julius-Peters)[6], 2–5 Nm[9], 2–3[10], 2 Nm (coarse HNF)[9], 4 Nm (ground HNF)[9], 2–4 Nm (HNF-C)[14], 2–4 Nm (HNF-S)[14], 2–4 Nm (HNF-E)[14], <0.5–2.5 Nm (ICI recrystallized HNF)[14], 3 (HNF-1, pilot-scale, isonated with ultrasound amplitude of 20 µm, X_{avg} = 300 µm, L/D_{avg} = 2.6)[14], 2 (HNF-2, pilot scale, isonated with ultrasound amplitude of 30 µm, X_{avg} = 320 µm, L/D_{avg} = 2.8)[14], 3 (BAM, HNF-C9)[15], 2–5 (general value for HNF batches)[15], 2 Nm (measured at ICT, 98.8–99.6 mass % purity)[16], 2–5 Nm (Aerospace Propulsion Products, Netherlands data, 98.8–99.6 mass % purity)[16], 2–20 Nm (BAM, range of results)[18], 24.7 cm (needles, BAM, Dixon's up and down method, 50% probability)[18], 11.6 cm (granules, BAM, Dixon's up and down method, 50% probability)[18], 7.5 Nm[18], 2–5 (BAM)[19], FoI = 33 (Rotter impact tester)[19], 4 (BAM)[20], 2–4[20]

<table>
<tr><td></td><td>Effect of ultrasound intensity during the cooling crystallization of HNF (sonocrystallization)[10]:

<table><tr><td>Ultrasound intensity (Tip amplitude, mu)</td><td>IS (J)</td></tr><tr><td>0</td><td>2</td></tr><tr><td>0.5</td><td>3</td></tr><tr><td>5.0</td><td>3</td></tr><tr><td>6.0</td><td>3</td></tr></table></td></tr>
<tr><td>FS [N]</td><td>28[1], 25[4], 24–36[10], 20 (coarse HNF)[9], 20 (ground HNF)[9], 16–36 (HNF-C)[14], 16–36 (HNF-S)[14], 16–36 (HNF-E)[14], 16–31 (ICI recrystallized HNF)[14], 12–14 (HNF-1, pilot scale, isonated with ultrasound amplitude of 20 µm, X_{avg} = 300 µm, L/D_{avg} = 2.6)[14], 12–16 (HNF-2, pilot-scale, isonated with ultrasound amplitude of 30 µm, X_{avg} = 320 µm, L/D_{avg} = 2.8)[14], 24 (HNF-3, isonated with ultrasound amplitude of 20 µm, X_{avg} = 320 µm, L/D_{avg} = 3.3)[14], 16 (BAM, HNF-C9)[15], 12–36 (general value for HNF batches)[15], 16 (measured at ICT, 98.8–99.6 mass % purity)[16], 18–36 (Aerospace Propulsion Products, Netherlands data, 98.8–99.6 mass % purity)[16], 12–36 (BAM range of results given in literature)[18], class 3 (needles)[18], class 3 (granules)[18], 24[18], 12–36 (BAM)[19], FoF = 1.3–1.5 (rotary friction tester)[19], 28 (BAM)[20], 16–36[20]

Effect of ultrasound intensity during the cooling crystallization of HNF (sonocrystallization)[10]:

<table><tr><td>Ultrasound intensity (tip amplitude, µ)</td><td>FS (N)</td></tr><tr><td>0</td><td>10</td></tr><tr><td>0.5</td><td>14</td></tr><tr><td>5.0</td><td>18</td></tr><tr><td>6.0</td><td>20</td></tr></table></td></tr>
<tr><td>ESD [J]</td><td>≥726 mJ[6], 4.5 (coarse HNF)[9], 4.5 (ground HNF)[9], ignition @ 4.5, no ignition @ 0.726[18], 1.71 (electric spark test, needles, Dixon’s up and down method, 50% probability)[18], 1.81 (electric spark test, granules, Dixon’s up and down method, 50% probability)[18], 726–4,500 mJ[19]</td></tr>
<tr><td>N [%]</td><td>38.25</td></tr>
<tr><td>$\Omega(CO_2)$ [%]</td><td>13.11</td></tr>
</table>

$T_{m.p.}$ [°C]

128 (DSC @ 10 °C/min)[1], 115–120[6], ≥116 (HNF-C, measured by black body radiation app.)[14], ≥115 (HNF-S, measured by black body radiation app.)[14], ≥115 (HNF-E, measured by black body radiation app.)[14], 124 (with dec.) (ICT-thermochemical database)[16], 120 (purity >98%)[17], values in range of 110–124 reported depending on the HNF purity[18], 123 (microthermocouple)[18], 128 (DSC @ 10 °C/min)[20], 128[20]

Onset of melting (DSC @ 10 °C/min, N_2 atmosphere, open Al cups)[15]: 131.0 (HNF-C9)[15], 130.8 (HNF-E8)[15]

Onset of melting (TG/DTA @ 10 °C/min, N_2 atmosphere, open Al cups)[15]: 131 (HNF-C9)[15], 132 (HNF-E8)[15]

Effect of using hydrazine hydrate (HZH) instead of purified anhydrous hydrazine (PAH) on HNF produced[19]:

HZ used	PAH	PAH	80% HZH	100% HZH	100% HZH	100% HZH	100% HZH
T_m (°C)	> 111	115.2	116.2	116.2	116.0	116.8	115.9

$T_{dec.}$ [°C]

131 (DSC @ 10 °C/min)[1], 124[2], 123[3], 121–129 (onset), 125–134 (peak) (DSC, ICI recrystallized HNF)[14]

Onset of dec. (DSC @ 10 °C/min, N_2 atmosphere, open Al cups)[15]: 134.3 (HNF-C9)[15], 134.2 (HNF-E8)[15]

onset of dec. (TG/DTA @ 10 °C/min, N_2 atmosphere, open Al cups)[15]: 134.5 (total mass decrease = 98.3 wt.%, HNF-C9)[15], 135.7 (total mass decrease = 97.4 wt.%, HNF-E8)[15]

Heating rate (°C/min)	T (°C)	Coarse HNF[9]	Ground HNF[9]
1	Onset	120.5	121.4
	Peak	121.7	121.8
	Extrapolated onset	121.1	121.7
2	Onset	123.5	124.1
	Peak	125.7	124.8
	Extrapolated onset	124.5	124.4
5	Onset	128.1	127.2
	Peak	130.0	128.3
	Extrapolated onset	128.7	127.6

TG-MS (two types of expts. performed: (i) scanning expts. = 1.8–4.5 mg sample, Al cup, 2 °C/min from 25–160 °C, MS run over entire range; (ii) isothermal = apparatus held @ constant T = 100 °C)[13]:

Experiment type	Total mass decrease (wt.%)	dec. *T* (°C)
Scanning	84	120–125
Scanning	100	120–125
Scanning	94	120–125
Isothermal	95	–

Thermal stability of aged and nonaged HNF[13]: ~135 (onset, exo, dec., DSC @ 10 °C/min, nonaged HNF, 3.4 mg sample)[13], ~145 (onset, exo, dec., DSC @ 10 °C/min, HNF aged @ 80 °C (slurry), 1.8 mg sample)[13]

DSC (@ various heating rates, HNF >98% purity, N_2 atmosphere)[17]:

Heating rate (°C/min)	First exotherm			Second exotherm			ΔH (J/g)
	T_i (°C)	T_{max} (°C)	T_f (°C)	T_i (°C)	T_{max} (°C)	T_f (°C)	
5	127.6	130.2	132.3	132.3	133.3	176.7	–2,301
10	131.9	135.8	137.9	137.9	138.2	178.3	–2,676
15	134.2	139.8	142.1	142.1	143.6	192.2	–2,389
20	135.6	142.1	144.2	144.2	145.1	190.8	–2,954
25	137.2	144.7	146.5	146.5	147.9	200.2	–2,535

DTA/TG (@ 10 °C/min, HNF >98% purity, static air atmosphere)[17]:

DTA					TG	
Peak details	T_i (°C)	T_{max} (°C)	T_f (°C)	Stages of dec.	*T* range (°C)	loss in weight (%)
First exotherm	130.7	133.5	135.5	First stage	105–142	72.5
Second exotherm	135.5	137	171.2	Second stage	142–210	24.5

	<90 °C no mass change observed but ~1.4% mass change @ 90–105 °C, rapid dec. >105 °C (TG @ 4 °C/min, air, *Hordijk*)[18], ~120 (strong exo, DTA @ 2 °C/min, *McHale*)[18], ~109 (weak exo), 110 (T_{max}, exo), 134 (T_{max}, exo), 139 (T_{max}, exo) (DTA @ 10 °C/min, *Shoyer*)[18], >131 (3 step dec., *Toshiyuki*)[18], 110–125 (onset, exo, range of values in DSC)[18], 131 (DSC @ 10 °C/min)[20], 132[20]		
ρ [g cm^{-3}]	1.88 (crystal @ 20 °C)[1], 1.86[6], 1.87[11], 1.03 (bulk ρ, HNF-1, pilot-scale, isonated with ultrasound amplitude of 20 µm, X_{avg} = 300 µm, L/D_{avg} = 2.6)[14], 1.05 (bulk ρ, HNF-2, pilot-scale, isonated with ultrasound amplitude of 30 µm, X_{avg} = 320 µm, L/D_{avg} = 2.8)[14], 0.96 (bulk ρ, HNF-3, isonated with ultrasound amplitude of 20 µm, X_{avg} = 320 µm, L/D_{avg} = 3.3)[14], 0.9 (bulk ρ, standard HNF-C produced under isonation)[14], 1.24 (tap ρ after 400 taps, HNF-1, pilot-scale, isonated with ultrasound amplitude of 20 µm, X_{avg} = 300 µm, L/D_{avg} = 2.6)[14, 19], 1.26 (tap ρ after 400 taps, HNF-2, pilot-scale, isonated with ultrasound amplitude of 30 µm, X_{avg} = 320 µm, L/D_{avg} = 2.8)[14, 19], 1.16 (tap ρ after 400 taps, HNF-3, isonated with ultrasound amplitude of 20 µm, X_{avg} = 320 µm, L/D_{avg} = 3.3)[14, 19], 1.06 (tap ρ after 400 taps, standard HNF-C produced under isonation)[14, 19], 1.872 (X-ray)[15], 1.87 (HNF-C9, He pycnometer @ 25 °C)[15], 1.83 (HNF-E8, He pycnometer @ 25 °C)[15], 1.869 (HNF-C9, Dodecane pycnometer @ 25 °C)[15], 1.846 (HNF-E8, Dodecane pycnometer @ 25 °C)[15], 1.846 (measured @ ICT)[16], 1.86 (Aerospace Propulsion Products, Netherlands data)[16], range of 1.86–1.93 reported[18], 1.88 (X-ray @ 25 °C)[20], 1.86–1.94 (@ 25 °C)[20]		
Heat of formation	–13 kcal mol^{-1}[1], –76.9 kJ/mol[2], –420 J/g[2], –18.4 ± 0.3 kcal mol^{-1} (assuming H_2O (l) formed on combustion, exptl.)[5], 7.6 kcal mol^{-1} (assuming H_2O (g) formed on combustion)[5], –72 kJ/mol (enthalpy of form.)[6], –17 kcal ($\Delta H_f°$)[8], -72 kJ mol^{-1} (ΔH_f)[11], –18.38 kcal/mol ($\Delta H_f°$, exptl.)[12], –18.20 kcal/mol ($\Delta H_f°$, calcd.)[12], –76.9 kJ/mol ($\Delta H_f°$)[16], –420.0 J/g ($\Delta H_f°$)[16], heat of formation ranges from –71––72 kJ/mol[18], –13 kcal/mol (ΔH_f, calcd., Gaussian 09)[20], 0.8–2.3 kcal/mol ($\Delta H_f°$)[20]		
Heat of combustion	5,796 J/g (measured @ ICT)[16], 5,824 J/g (Aerospace Propulsion Products, Netherlands data)[16, 18]		
	Calcd. (EXPLO5 5.02)	Lit. values	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]	5,451 (@ 1.938 g cm^{-3})[5] 5,452 (@ 1.930 g cm^{-3})[5] 5,447 (@ 1.890 g cm^{-3})[5] 5,443 (@ 1.860 g cm^{-3})[5]	5,579 (calcd., ICT-thermodynamic code)[2] 5,579 (calcd., ICT thermodynamic code) [H_2O (g)][16]	
T_{ex} [K]	4,085 (@ 1.938 g cm^{-3})[5] 4,057 (@ 1.930 g cm^{-3})[5] 4,086 (@ 1.890 g cm^{-3})[5] 4,107 (@ 1.860 g cm^{-3})[5]		

$p_{C\text{-}J}$ [kbar]	380 (@ 1.938 g cm^{-3})[5] 368 (@ 1.930 g cm^{-3})[5] 354 (@ 1.890 g cm^{-3})[5] 344 (@ 1.860 g cm^{-3})[5]	35.4 (calcd.)[1] 35.4 (calcd., EXPLO5 V5.05)[20]	
VoD [m s^{-1}]	9,286 (@ 1.938 g cm^{-3})[5] 9,146 (@ 1.930 g cm^{-3})[5] 9,028 (@ 1.890 g cm^{-3})[5] 8,948 (@ 1.860 g cm^{-3})[5]	8,858 (calcd.)[1] 8,858 (no ρ specified, calcd., EXPLO5 V5.05)[20]	
V_0 [L kg^{-1}]	826 (@ 1.938 g cm^{-3})[5]	568 (calcd., ICT-thermodynamic code)[2, 16]	

Critical diameter [cm]	<10 mm (test sample = 91% HNF, 9% wax, ρ = 1.680 g cm^{-3})[18], <10 mm[19]
Shock sensitivity	3 GPa (ϕ = 30 mm, test sample = 91% HNF, 9% wax, ρ = 1.680 g cm^{-3})[18]
5 s explosion T [°C] Ignition T [°C] Autoignition T [°C]	400 (self-ignition)[8], 260 (deflagration)[8] 131 (@ 5 °C/min, Wood's metal bath, HNF lot 1, APP, Netherlands, needle-like, mean particle size = ~240 µm, 0.2 g sample)[16], 129 (@ 5 °C/min, HNF lot 2, APP, Netherlands, needle-like, Wood's metal bath, 0.2 g sample)[16], 129 (@ 5 °C/min, HNF lot 3, APP, Netherlands, spherical, mean particle size = 76 µm, Wood's metal bath, 0.2 g sample)[16]
Thermal stability	Stable @ 77 °C for 40 h[7] Mass loss (%) as function of time (d) @ various T (°C) for HNF lot 1 (APP, Netherlands, needle-like, mean particle size = ~240 µm)[16]: @ 50 °C: 0.05%/7 d, 0.1/14, 0.2/25, 0.2/37.5, 0.2/60, 0.4/89, 0.4/114, 0.4/136[16] @ 60 °C: 0.1%/7 d, 0.2/14, 1.0/25, 1.9/37.5, 3/45[16] @ 70 °C: 0.5%/7 d, 1.4/14, 4.5/22.5[16] @ 80 °C: 0.5%/1 d, 1.5/2.5, 3.5/5[16] ML (%) as function of time (d) @ various T (°C) for HNF lot 2 (APP, Netherlands, needle-like)[16]: @ 65 °C: 0%/0 d, 0.05/2, 0.1/4, 0.2/6, 0.3/9, 0.5/12, 0.75/16, 1.0/17[16]

@ 70 °C: 0%/0 *d*, 0.05/2, 0.3/4, 0.5/6, 0.75/8, 1/10, 1.5/12, 2.7/16[16]
@ 75 °C: 0%/0 *d*, 0.2/2, 1.0/4, 2.5/6, 4.5/7[16]

ML (%) as function of time (d) @ various T (°C) for HNF lot 3 (APP, Netherlands, spherical, mean particle size = 76 µm)[16]:
@ 65 °C: 0%/0 *d*, 0.1/2, 0.3/4, 0.5/6, 0.75/9, 0.9/11, 1.0/12, 1.3/14, 1.75/18[16]
@ 70 °C: 0%/0 *d*, 0.1/2, 0.5/4, 1.0/6, 1.3/8, 1.6/9, 1.9/10, 2.25/11, 2.5/12, 3/13, 4.25714[16]
@ 75 °C: 0%/0 *d*, 0.3/2, 0.7/3, 1.25/4, 2.3/5, 4.5/6[16]

Decomposition rate of HNF and HNF stabilized by aldehydes @ 90 °C under vacuum, cc gas evolved per g sample, + = high dec. of >28 cc gas/g[21]:

Specimen	Decomposition, cc, gas/g @ STP in		
	20 h	30 h	40 h
Untrated HNF	28	28 +	28 +
HNF + 3% 2,4-dihydroxybenzaldehyde	0	2	23
HNF + 3% benzaldehyde	0	1	5

Vacuum stability test [cm^3/h]

0.22 mL/g (coarse HNF, Hg column, 48 h @ 60 °C)[9]†, 0.55 mL/g (ground HNF, Hg column, 48 h @ 60 °C)[9] †
†VST is higher in ground than coarse (received) HNF probably because of solvent residue evaporation due to solvent being used in grinding)
≤0.5 mL/g (60 °C, 48 h, HNF-C)[14], ≤1.8 mL/g (60 °C, 48 h, HNF-S)[14], ≤0.2 mL/g (60 °C, 48 h, HNF-E)[14], 0.4–1.3 mL/g (60 °C, 48 h, ICI recrystallized HNF)[14], 3.4–5.4 mL/g (80 °C, 24 h, ICI recrystallized HNF)[14], 0.92 mL/g (70 °C, 48 h, sealed and evacuated test tube, HNF-E8)[15], 0.57 mL/g (70 °C, 48 h, sealed and evacuated test tube, HNF-C9)[15]

@ 60 °C, ultrasound isonation during cooling crystallization, ultrasound vibrations up to 8 µm[14]:

Time (h)	Gas production (mL/g)	Time (h)	Gas production (mL/g)
5	~ 0.5	25	~ 0.8
7	~ 0.6	31	~ 0.9
23	~ 0.7	48	~ 1.1

@ 60 °C, ultrasound no isonation during re-crystallization[14]:

Time (h)	Gas production (mL/g)	Time (h)	Gas production (mL/g)
5	~ 0.21	25	~ 0.29
7	~ 0.22	31	~ 0.3
23	~ 0.28	48	~ 0.36

@ 80 °C, ultrasound isonation during cooling crystallization, ultrasound vibrations up to 8 µm[14]:

Time (h)	Gas production (mL/g)	Time (h)	Gas production (mL/g)
5	~ 0.5	~ 70	~ 1.8
24	~ 1.2	100	~ 3.1
50	~ 1.3		

@ 80 °C, no ultrasound isonation during recrystallization[14]:

Time (h)	Gas production (mL/g)	Time (h)	Gas production (mL/g)
5	~ 1.0	~ 70	~ 2.3
24	~ 1.2	100	~ 5.4
~50	~ 1.8		

0.082 mL/g (@ 60 °C, 48 h, 2 g sample, HNF lot 1, APP, Netherlands, needle-like, mean particle size = ~240 µm)[16], 0.084 mL/g (@ 60 °C, 48 h, 2 g sample, HNF lot 2, APP, Netherlands, needle-like)[16], 0.072 mL/g (@ 60 °C, 48 h, 2 g sample, HNF lot 3, APP, Netherlands, spherical, mean particle size = 76 µm)[16], 1.10 mL/g (@ 80 °C, 40 h, extrapolated, HNF lot 1, APP, Netherlands, needle-like, mean particle size = ~240 µm)[16], 1.13 mL/g (@ 80 °C, 40 h, extrapolated, HNF lot 2, APP, Netherlands, needle-like)[16], 0.95 mL/g (@ 80 °C, 40 h, extrapolated, HNF lot 3, APP, Netherlands, spherical, mean particle size = 76 µm)[16], 4.4 mL/g (@ 90 °C, 40 h, extrapolated, HNF lot 1, APP, Netherlands, needle-like, mean particle size = ~240 µm)[16], 4.5 mL/g (@ 90 °C, 40 h, extrapolated, HNF lot 2, APP, Netherlands, needle-like)[16], 3.8 mL/g (@ 90 °C, 40 h, extrapolated, HNF lot 3, APP, Netherlands, spherical, mean particle size = 76 µm)[16], 17.5 mL/g (@ 100 °C, 40 h, extrapolated, HNF lot 1, APP, Netherlands, needle-like, mean particle size = ~240 µm)[16], 17.9 mL/g (@ 100 °C, 40 h, extrapolated, HNF lot 2, APP, Netherlands, needle-like)[16], 15.4 mL/g (@ 100 °C, 40 h, extrapolated, HNF lot 3, APP, Netherlands, spherical, mean particle size = 76 µm)[16]

Gas evolution values of 2–10 cc/g @ 60 °C, 48 h reported[18], excessive gas evolution attributed to impurities[18], 0.1–0.5 cc/g for recryst. HNF @ 60 °C, 48 h[18]

Effect of using hydrazine hydrate (HZH) instead of purified anhydrous hydrazine (PAH) on HNF produced[19]:

HZ used	PAH	PAH	80% HZH	100% HZH	100% HZH	100% HZH	100% HZH
VTS @ 60 °C, 48 h (mL/g)	<2.5	1.0	0.34	0.34	0.28	0.29	0.41
VTS @ 80 °C, 100 h (mL/g)		stopped after 75 h because 20 mL/g already evolved	2.8	3.8	6.0	2.4	5.2

VTS @ 90 °C for various types of HNF[19]:

gas evolution (mL/g)	Time to specified gas evolution (h) for HNF type				
	US Patent 1	US Patent 2	26	1	23
8	14.6	15.3	30.2	34	34.3
20	17.7	20	–	–	46.7
23.3	19	–	–	–	48

Experimentally determined activation energy for the slow dec. of HNF[19]:

HNF batch	VTS gas production	Time until gas production is reached, h			E (kJ/mol)	cc
		60 °C	80 °C	90 °C		
23	3 mL/g	2,675	102	25	157.2	0.9998
	Run away	4,000	190	50	147.3	0.9999
1	3 mL/g	2,225	99	20	157.0	0.9992
	Run away	3,000	170	35	147.8	0.9980

<table>
<tr><td>Burn rate [mm/s]</td><td>Pressed neat HNF: burning rate exponent $n = 0.95$ @ pressure <2 MPa[19], $n = 0.85$ @ pressures >2 MPa–10 MPa[19]; burning rate exponent $n = 0.92$ @ pressure <2 MPa (<i>Sinditskii</i>)[19], $n = 0.76$ @ pressures >2 MPa–10 MPa (<i>Sinditskii</i>)[19]</td></tr>
<tr><td>Solubility [g/mL]</td><td>Reasonable solubility only obtained in polar solvents[10], insoluble in (cyclo)alkanes or aromates (e.g., toluene, xylene)[10], solubility of HNF generally increases with increasing solvent polarity[10], crystals obtained from MeOH, EtOH, 1-propanol, 2-propanol[10], easily soluble in H_2O[16], sparingly soluble in most common organic solvents[18] except alcohols in which it is moderately soluble[18], highly soluble in H_2O (112.21%)[18]

T dependence of solubility[10]:

<table>
<tr><td rowspan="2">Solvent</td><td colspan="2">Temperature (°C)</td></tr>
<tr><td>20 °C</td><td>40 °C</td></tr>
<tr><td>MeOH</td><td>~ 20 wt.%</td><td>~ 30 wt.%</td></tr>
<tr><td>EtOH</td><td>~ 8 wt.%</td><td>~ 12 wt.%</td></tr>
<tr><td>1-propanol</td><td>~ 1 wt.%</td><td>~ 4 wt.%</td></tr>
<tr><td>2-propanol</td><td>~ 1 wt.%</td><td>~ 4 wt.%</td></tr>
</table>

Solubility in g/100 g solvent[18]: 22.28 (methanol)[18], 5.98 (ethanol)[18], 1.14 (2-propanol)[18], 1.12 (ethyl acetate)[18], 112.21 (H_2O)[18]

Mole fraction (x) solubility in MeOH or EtOH at various temperatures[20]:

<table>
<tr><td>T (°C)</td><td>MeOH</td><td>EtOH</td></tr>
<tr><td>10</td><td>0.1</td><td>0.025</td></tr>
<tr><td>20</td><td>0.14</td><td>0.04</td></tr>
<tr><td>30</td><td>0.175</td><td>0.06</td></tr>
<tr><td>40</td><td>0.225</td><td>0.08</td></tr>
<tr><td>50</td><td>0.3</td><td>0.1</td></tr>
</table>
</td></tr>
<tr><td>Hygroscopicity</td><td>Rel. low hygroscopicity[7], hygroscopic[11], easily soluble in H_2O[16], nonhygroscopic[17, 18]</td></tr>
<tr><td>Compatibility</td><td>Incompatible with HTPB[18] and isocyanates[18], compatible with GAP[18] and Al[18], HNF is stabilized by ~1–5 wt.% of benzaldehyde, dihydroxybenzaldehyde or a mixture of the two[21]</td></tr>
</table>

<table>
<tr><td>Activation energy for dec. [kJ/mol]</td><td>166 (intrinsic dec. reaction)[16], 139 (intrinsic dec. reaction)[16], 132 (intrinsic dec. reaction)[16], 159 (autocatalytic reaction)[16], 128 (autocatalytic reaction)[16], 117 (autocatalytic reaction; different values in[16] are for different HNF batches)[16], 150[17], 25 kcal/mol (for dec. of melt/foam layer, Brill)[18]

Experimentally determined activation energy for the slow dec. of HNF[19]:
<table>
<tr><th rowspan="2">HNF batch</th><th rowspan="2">VTS gas production</th><th colspan="3">Time until gas production is reached, h</th><th rowspan="2">E (kJ/mol)</th><th rowspan="2">cc</th></tr>
<tr><th>60 °C</th><th>80 °C</th><th>90 °C</th></tr>
<tr><td rowspan="2">23</td><td>3 mL/g</td><td>2,675</td><td>102</td><td>25</td><td>157.2</td><td>0.9998</td></tr>
<tr><td>Run away</td><td>4,000</td><td>190</td><td>50</td><td>147.3</td><td>0.9999</td></tr>
<tr><td rowspan="2">1</td><td>3 mL/g</td><td>2,225</td><td>99</td><td>20</td><td>157.0</td><td>0.9992</td></tr>
<tr><td>Run away</td><td>3,000</td><td>170</td><td>35</td><td>147.8</td><td>0.9980</td></tr>
</table>
</td></tr>
<tr><td>Energy release during dec. [kJ/kg]</td><td>4,700 (DSC, Hordijk)[18], 4800 (due to two exotherms, DSC, Hatano)[18]</td></tr>
<tr><td>Drop ball test (cm)</td><td>Direct (50% probability): 2.75 cm (needle), 4.43 cm (granule)[18]; indirect (50% probability): 0.25 cm (needle), 0.47 cm (granule)[18]</td></tr>
<tr><td>Surface T (T_s) [K]</td><td>Temperatures during burning in relation to pressure (pressed, neat HNF)[19]: 530 K @ 0.1 MPa, 560 K @ 0.2 MPa, 620 K @ 0.5 MPa, 675 K @ 1.0 MPa[19], 553 K @ 0.1 MPa (loosely packed HNF, McHale)[19], 615 K ± 11 K @ 0.1 MPa (Sinditskii)[19], 750 K ± 10 K @ 2 MPa (Sinditskii)[19]</td></tr>
<tr><td>$\Delta_{diss}H$ [kJ/mol]</td><td>19.77 (in MeOH)[20], 25.35 (in EtOH)[20]</td></tr>
</table>

	HNF[5]
Chemical formula	$CH_5N_5O_6$
Molecular weight [g mol^{-1}]	183.10
Crystal system	Monoclinic
Space group	$P\,2_1/\,n$ (no. 14)
a [Å]	8.044(8)
b [Å]	5.4420(5)
c [Å]	14.5015(12)
α [°]	90
β [°]	98.785(8)
γ [°]	90

V [Å^3]	627.4(1)
Z	4
ρ_{calc} [g cm^{-3}]	1.938
T [K]	100

A detailed description of crystal morphology with respect to recrystallization is given in[10]

Comparison of the four commercial grades of HNF[14, 19]:

Parameter	HNF-C[14, 19]	HNF-S[14, 19]	HNF-E[14, 19]	HNF-P[14, 19]
Process	(Obtained by cooling crystallization; soln. of HNF in MeOH is cooled below saturation point, seed crystals introduced)	(Solvent/ nonsolvent recryst. process; HNF dissolved in MeOH (solvent) and added to methylene chloride (antisolvent))	(Evaporative crystallization; NF dissolved in isopropyl alcohol, heated then isopropanol vaporized under vacuum while HNF-E crystallizes)	(Obtained when hydrazine is added to nitroform/ dichloroethane mixture)
$[HNF]_{acid}$ [wt.%]	99.8–100.8	98.8–99.6	99.0–100.3	
$[HNF]_{HZ}$ [wt.%]	97.9–100.0	97.2–99.6	97.8–99.3	
T_m (black body radiation apparatus) [°C]	≥116 (<116)	≥115	≥115	>115
VTS (60 °C, 48 h) [mL/g]	≤0.5 (<0.5)	≤1.8	≤0.2	<0.5
L/D	≤8 (<8)	≤8	–	1–4
X_{50} [µm]	400–900 (200–1,000)	50–150	–	300
X_{10}/X_{50}	≥0.5	≥0.6	–	
X_{90}/X_{50}	≤1.5	≤1.4	–	
FS (BAM) [N]	16–36	16–36	16–36	
IS (BAM)[Nm]	2–4	2–4	2–4	
ρ_{tap} [kg m^{-3}]	(800–1,000)	400–600		

X_{10} = particle size for which 10% of total size distribution is smaller; X_{50} = particle size for which 50% of total size distribution is smaller, particle size based on equivalent spherical diameter; X_{90} = particle size for which 90% of total size distribution is smaller; L/D = length over diameter ratio = aspect ratio; $[]_{acid}$ = conc. based on acid content; $[]_{HZ}$ = conc. based on HZ content

Some properties of cocrystallized HNF[19]:

Property	Cocrystallized HNF			Ref. data for HNF
	HNF	HNF + 2% stabilizer	HNF + 2% coating	
L/*D*	~1	~1	1–2	1–4 (HNF-C and HNF-S)
D (µm)	~10	~2	~3.5–~7	>40
VTS (60 °C, 48 h), mL/g	0.37	0.35	0.75	<1.8
VTS (80 °C, 24 h), mL/g	1.8	1.3	3.3	n/a
N_2H_4, wt.%	97.6	96.7	96.1	97.2–100.0
H_3O^+, wt.%	100.3	101.6	98.7	98.8–100.8
Onset melt, °C	127.5	129	118	129
Onset dec., °C	128.9	128.9	127	129
FS, N	20	35	29	14–32
IS, Nm	2.5	2	3	>2

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[18] P. S. Dendage, D. B. Sarwade, S. N. Asthana, H. Singh, *J. Energet. Mater.*, **2001**, *19*, 41–78.
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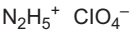
Hydrazinium perchlorate

Name [German, acronym]: Hydrazinium perchlorate, hydrazine Perchlorate [HP, HPC]

Main (potential) use: Oxidizer for solid propellants[1]

Structural formula:



	Hydrazinium perchlorate	
Formula	$H_5N_2O_4Cl$	
Molecular mass [g mol^{-1}]	132.50	
Appearance at RT	White crystalline solid[6]	
IS [J]	2 Nm[2], $H_{50\%}$ = 1.2 cm (2 kg mass, B.M.)[6], $H_{50\%}$ = 32 cm (5 kg mass, Rotter)[6], more sensitive than PETN, but sensitivity depends markedly on water content[6]	
FS [N]	>10[2]	
N [%]	24.15	
Ω(CO_2) [%]	+18.1	
$T_{m.p.}$ [°C]	144[2], 142.4[3], 131–132[7, 11], 137–138[10], $N_2H_5ClO_4 \bullet {}^1/_2H_2O$ obtained from aq. solns. has mpt. = 85[10], 142[6]	
$T_{dec.}$ [°C]	145 (begins), complete dec. by 230[7], dec. occurs near mpt. (142 °C)[6]	
ρ [g cm^{-3}]	1.84[4], 1.939[7]	
Heat of formation	–179.5 kJ/mol ($\Delta H_f°$, exptl.)[4], –1,331 kJ/kg (enthalpy of form.)[2], 40.69 ± 0.36 kcal mol^{-1} ($\Delta H_f°$) [7], 42.9 ± 0.2 kcal/mol ($\Delta H_f°$)[7], –42.05 kcal/mol (ΔH_f, (s))[6], –44.46 kcal/mol (ΔH_f, (s))[6], –40.62 kcal/mol ($\Delta H_f°$)[12], –41.78 kcal/mol ($\Delta H_f°$, calcd.)[12]	
	Calcd. (EXPLO5 6.03)	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]	3,069	3,690 [H_2O (l)][2] 3,033 [H_2O (g)][2]
T_{ex} [K]	2,640	2,275 ± 50[5]
$p_{C\text{-}J}$ [GPa]	26.6	
VoD [m s^{-1}]	7,990 (@ 1.939 g cm^{-3})	
V_0 [L kg^{-1}]	922	838[2] 864[7]

<table>
<tr><td>Trauzl test [cm^3, % TNT]</td><td>120% TNT[9], 113% PA[7], 122% TNT[7]</td></tr>
<tr><td>Shock sensitivity</td><td>Similar to that of MF[10]</td></tr>
<tr><td>5 s explosion T [°C]
Ignition T [°C]</td><td>277–283 (0.2 g sample heated from 100 °C @ 20 °C/min)[6], 238[6]</td></tr>
<tr><td>Thermal stability</td><td>Weight loss on holding a sample @ given T for 6 min[6]: 0.3% @ 180 °C[6], 5.4% @ 240 °C[6], rapid combustion @ 250 °C[6]

97–99% used for sublimation from melt to cold finger @ 180–235 °C showed no dec.[6]</td></tr>
<tr><td>Burn rate [mm/s]</td><td>Pure HP burns smoothly when ignited[6], powder samples packed into glass tube (1.05 cm inside diameter) did not ignite using white hot wire @ atmospheric pressure, sample only melted and ignited on surface layer[6]

Effect of catalysts on combustion of Hydrazinium perchlorate at 1 atm[6]:
<table>
<tr><th>Catalyst</th><th>%</th><th>Density (g/cm^3)</th><th>Burn rate (cm s^{-1})</th></tr>
<tr><td>MnO_2</td><td>5</td><td>1.27</td><td>0.13</td></tr>
<tr><td>CoO</td><td>5</td><td>1.29</td><td>0.85</td></tr>
<tr><td>Cu_2Cl_2</td><td>5</td><td>1.27</td><td>1.5</td></tr>
<tr><td>$Cu_2Cl_2 \bullet 2H_2O$</td><td>5</td><td colspan="2">Does not burn steadily</td></tr>
<tr><td rowspan="3">MgO</td><td>2</td><td>1.90</td><td>0.26</td></tr>
<tr><td>5</td><td>1.91</td><td>0.31</td></tr>
<tr><td>10</td><td>1.89</td><td>0.35</td></tr>
<tr><td rowspan="3">Copper chromite</td><td>2.5</td><td>1.13</td><td>Does not deflagrate</td></tr>
<tr><td>5</td><td>1.10</td><td>1.20</td></tr>
<tr><td>5</td><td>1.93</td><td>0.72</td></tr>
<tr><td rowspan="2">$K_2Cr_2O_7$</td><td>2.5</td><td>1.17</td><td>Does not deflagrate</td></tr>
<tr><td>5</td><td>1.19</td><td>0.75</td></tr>
<tr><td>CaO</td><td>2</td><td>1.31</td><td>0.12</td></tr>
</table></td></tr>
<tr><td>Solubility [g/mL]</td><td>23.6 g/100 g H_2O @ 0 °C[6], 68.9 g/100 g H_2O @ 40 °C[6]</td></tr>
<tr><td>Heat of vaporization [kcal/mol]</td><td>29.2[6]</td></tr>
<tr><td>Heat of fusion [kcal/mol]</td><td>3.84[6], 1.68[6]</td></tr>
</table>

	HP[8]
Chemical formula	$H_5N_2O_4Cl$
Molecular weight [g mol^{-1}]	132.50
Crystal system	Monoclinic
Space group	*C* 2/ *c* (no. 15)
a [Å]	14.412(7)
b [Å]	5.389(5)
c [Å]	12.797(3)
α [°]	90
β [°]	113.09(5)
γ [°]	90
V [Å^3]	914.2707
Z	8
ρ_{calc} [g cm^{-3}]	
T [K]	

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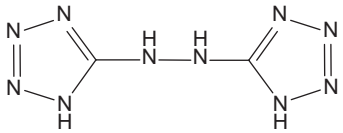
5,5′-Hydrazotetrazole

Name [German, acronym]: 5,5′-Hydrazodi-(1*H*)-tetrazole, 1,2-bis(5,5′-tetrazolato) hydrazine [5,5′-hydraotetrazol, 5,5′-HzTz, HAT]

Main (potential) use:

Structural formula:



	HAT		
Formula	$C_2H_4N_{10}$		
Molecular mass [g mol^{-1}]	168.12		
Appearance at RT	White amorphous powder[1]		
IS [J]	No fire level = 0.0 cm, W_{50} = 12.5 cm (ball weight = 28 g, ball weight method)[1], >50 cm (ball and disk test)[3], $H_{50\%}$ = 20 cm[3], 32 cm (2.5 kg mass)[4]		
FS [N]	No fire level = 2.9 ms^{-1}, W_{50} = 3.2 ms^{-1} (load weight = 4 kg, friction pendulum apparatus)[1], >3.7 m/s (Emery paper test)[3]		
ESD [J]	Energy required for initiation = n/s ((not sensitive)gap between needle and vial = 2 cm, based on the variable gap technique)[1], ignitions @ 0.045 J (standard test)[3], ignition @ 42 µJ but not @ 32 µJ (test no. 7)[3]		
N [%]	83.31		
Ω(CO_2) [%]	−57.10		
$T_{m.p.}$ [°C]			
$T_{dec.}$ [°C]	521 K (DSC, 8 °C/min, Al_2O_3 added as dilutent to prevent explosions, non-isothermal conditions, steady flow rate of He/N_2, heat of dec. = 2,089.2 ± 59.5 kJ kg^{-1})[1], 218 (onset, DSC @ 10 °C/min, with ignition @ 238 °C)[3]		
ρ [g cm^{-3}]	1.01 (bulk ρ)[1], 1.85 (calcd.)[3]		
Heat of formation			
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{ex}U^{o}$ [kJ kg^{-1}]			
T_{ex} [K]			
$p_{C\text{-}J}$ [kbar]			

VoD [m s^{-1}]			
V_0 [L kg^{-1}]			
Lead plate test	Charge weight (g): 35(F) (full initiation), 30(P) (partial initiation), 25(P) (partial initiation), 20(N) (no initiation)[1]		
5 s explosion *T* [°C] Ignition *T* [°C] Explosion *T* [°C]	 238[3], 215 (explodes in *T* of *I* test)[3], 239 (hot bar ignition *T*)[4] 229[3]		
Thermal stability	78.0–79.0% weight loss in TG[1]		
Vacuum stability test [cm^3/h]	6.9 @ 120 °C/40 h[3], 1.7 cc gas/48 h/100 °C[4]		
Blast wave characteristics	(blast wave) peak overpressure P_{max} = 3.4 kPa (mean value)[2], (blast wave) positive phase impulse I^+ = 0.43 Pa s (mean value)[2] (loose filled into mild steel test units 84.6 × 2.5 × 2.5 cm), 0.9 cm hole diameter, sealed with a cork disk and adhesive, mass or material = 200–1,000 g, initiated with an ICI type "E" fuzehead)[2]		

[1] G. O. Reddy, A. K. Chatterjee, *J. Hazard. Mater.*, **1984**, *9*, 291–303.
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[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**.
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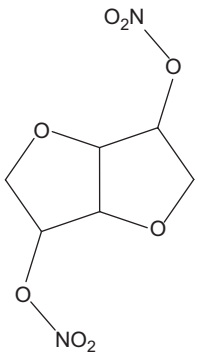
I

Isosorbitol dinitrate

Name [German, acronym]: Isosorbitol dinitrate, isosorbide dinitrate, 1,4:3,6-dianhydro-D-glucitol-2,5-dinitrate, 1,4;3,6-dianhydro-2,5-dinitrosorbitol, dinitrosorbide, isosorbide dinitrate, Carvanil, Carvasin, Cedocard, Cardis, Harrical, Iso-Bid, Isoket, Isosorbid, Isordil, Laserdil, Maycor, Rigedal, Sorbangil, Sorbidilat, Sorbitrate, Sorquad, Vascardin, Vasorbate [isosorbitdinitrat, ISDN]

Main (potential) use: pharmacy (angina pectoris)

Structural formula:



	Isosorbitol dinitrate
Formula	$C_6H_8N_2O_8$
Molecular mass [g mol^{-1}]	236.14
Appearance at room temperature	White crystals[4], hard colorless crystals[7]
IS [J]	15 Nm[1], 200 cm (0 sample fired, 5 kg mass)[5]
FS [N]	>160[1], 36 kg load (0 sample fired, Julius-Peters)[5]
N [%]	11.86
$\Omega(CO_2)$ [%]	−54.2

https://doi.org/10.1515/9783110672565-009

$T_{m.p.}$ [°C]	70 (dec.)[1], 69–70[5], 340 K (pure ISDN, DSC @ 10 K/min, nonisothermal conditions, N_2 atmosphere, crimped in Al pans with hole in lid, 2–4 mg sample)[4], 335.0 K (crude ISDN, DSC @ 10 K/min, nonisothermal conditions, N_2 atmosphere, crimped in Al pans with hole in lid, 2–4 mg sample)[4], 72 (endo, DSC, peak max)[5]
$T_{dec.}$ [°C]	70[1], 443.0 K (onset, sharp dec. exo), 467.0 K (peak *T*), 482.0 K (end *T*) (pure ISDN, DSC @ 10 K/min, non-isothermal conditions, N_2 atmosphere, crimped in Al pans with hole in lid, 2–4 mg sample)[4], 427.0 K (onset, broad dec. exo), 452 K (peak *T*), 480.0 K (end *T*) (crude ISDN, DSC @ 10 K/min, nonisothermal conditions, N_2 atmosphere, crimped in Al pans with hole in lid, 2–4 mg sample)[4], 72 (endo, DSC, peak max)[5], 223 (exo peak max, sharp peak, DSC)[5], 70[7] Thermal stability – effect of heating rate[4]:

Material	Heating rate (K/min)	Peak *T* (K)
Pure ISDN	5	458.0
Pure ISDN	10	467.0
Pure ISDN	20	475.0
Pure ISDN	40	481.0
Crude ISDN	5	440.0
Crude ISDN	10	452.0
Crude ISDN	20	472.0
Crude ISDN	40	483.0

ρ [g cm^{-3}]	1.65 ± 0.1 (@ 293.15 K)[2]		
Heat of formation			
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{ex}U^{o}$ [kJ kg^{-1}]			
T_{ex} [K]			
$p_{C\text{-}J}$ [GPa]			
VoD [m s^{-1}]			5,300 (@ 1.08 g cm^{-3})[1] 3,921 (@ 0.82 g cm^{-3}, crude ISDN, 25 mm plastic tube, fired with No. 6 detonator)[4]

			3,849 (@ 0.87 g cm^{-3}, crude ISDN and 5% H_2O, 25 mm plastic tube, fired with no. 6 detonator)[4] Cap failed (@ 0.92 g cm^{-3}, crude ISDN and 10% H_2O, 25 mm plastic tube, fired with no. 6 detonator)[4] Cap failed (@ 1.04 g cm^{-3}, crude ISDN and 20% H_2O, 25 mm plastic tube, fired with no. 6 detonator)[4] 4,021 (@ 0.49 g cm^{-3}, pure ISDN, 25 mm plastic tube, fired with no. 6 detonator)[4] 3,129 (@ 0.60 g cm^{-3}, crude ISDN and 10% H_2O, 25 mm plastic tube, fired with no. 6 detonator)[4] Cap failed (@ 0.96 g cm^{-3}, crude ISDN and 25% H_2O, 25 mm plastic tube, fired with no. 6 detonator)[4]
V_0 [L kg^{-1}]			

Trauzl test [cm^3, % TNT]	304 mL (10 g sample)[5], 311 cm^3[6]
Ballistic mortar test	64.6% (10 g sample, Al used as wrapper)[5]
5 s explosion T [°C] Explosion T [°C]	180–185[5]
Abel heat test	1 h @ 60 °C[5]
Thermal stability	TG, 10 K/min[4]: Material | T range (K) | Weight loss (%) Pure ISDN | 413.0–473.0 | 90.5 Crude ISDN | 393.0–493.0 | 84.8
Activation energies to decomposition [kJ/mol]	E_{act} = 87.36 (crude ISDN, DSC, Ozawa's method)[4], E_{act} = 174.70 (pure ISDN, DSC, Ozawa's method)[4], E_{act} = 68.75 (crude ISDN, TG, 10 K/min, Ozawa's method)[4], E_{act} = 158.80 (pure ISDN, TG, 10 K/min, Ozawa's method)[4]

Heat of decomposition [J/g]	2319.0 (100% ISDN, DSC, 10 K/min, nonisothermal conditions, N_2 atmosphere, crimped in Al pans with hole in lid, 2–4 mg sample)[4]
Solubility [g/mL]	Sparingly soluble in water (1.0 g dissolves in 900 mL H_2O)[7], freely soluble in common organic solvents such as EtOH, Et_2O and acetone[7]

	Isosorbitol dinitrate[3]
Chemical formula	$C_6H_8N_2O_8$
Molecular weight [g mol^{-1}]	236.14
Crystal system	Orthorhombic
Space group	$P22_12_1$ (no. 18)
a [Å]	5.7535(2)
b [Å]	10.9393(5)
c [Å]	14.6599(5)
α [°]	90
β [°]	90
γ [°]	90
V [Å^3]	922.683
Z	4
ρ_{calc} [g cm^{-3}]	1.7
T [K]	295

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[2] Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© **1994–2017** ACD/Labs).
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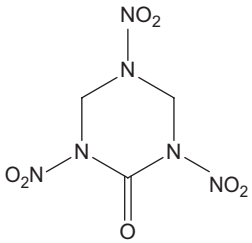
K

Keto-RDX

Name [German, acronym]: 1,3,5-Trinitro-1,3,5-triazacyclohexane-2-one, 2-oxo-1,3,5-trinitro-1,3,5-triazacyclohexane, 2-oxo-1,3,5-trinitro-1,3,5-triazacyclohexane, 1,3,5-trinitro-1,3,5-triazinan-2-one, 1,3,5-trinitro-hexahydro-1,3,5-triazin-2(1*H*)-one [Keto-RDX, K-6]

Main (potential) use: Fuel component in inflatable vehicle occupant protection devices with reduced smoke[5]

Structural formula:



	K-6
Formula	$C_3H_4N_6O_7$
Molecular mass [g mol^{-1}]	236.10
Appearance at room temperature (RT)	White crystalline solid[5], colorless crystals[13, 14], white solid[14, 15]
IS [J]	11 cm (lower explosive limit, Kasta hammer, 5 kg mass)[2], 27 cm (upper explosive limit, Kasta hammer, 5 kg mass)[2], $H_{50\%}$ = 25 cm (micro-K-6, BAM, 5 kg mass)[5], $H_{50\%}$ = 30 cm (nano-K-6, BAM, 5 kg mass)[5], 1.5 ± 0.5 Nm (BAM)[9], 12.5 (micro-K-6)[12], 15.0 (nano-K-6)[12], 15 cm[14], 19 cm (K-6/Viton A, 95:5)[14], $H_{50\%}$ = 7.5 ± 2.5 cm (2 kg mass, Bruceton method, BAM)[15], A_{d1} = 92%, LL = 0.5 m, $A_{50\,d1}$ = 1.4 m, $A_{50\,d2}$ = 1.3[18]
FS [N]	9.6 kg (lower sensitivity limit, BAM)[2], 16 kg (upper sensitivity limit, BAM)[2], 12 kgf (nanocrystalline-K-6)[5], 6.4 kgf (micro-K-6)[5], 50 (micro-K-6, 1,000 particle size)[8], 125 (micro-K-6, 1,000 particle size)[8], 75 (nano-K-675 particle size)[8], 10.8 ± 2.4 kp[9], 64 (50% load, micro-K-6)[12], 120 (50% load, nano-K-6)[12], 4.2 kg[14], 4.2 kg (K-6/Viton A, 95:5)[14], 10.8 ± 2.4 kp (50% level, Julius–Petri)[15], $P_{fr.LL}$ = 250 MPa[18], $P_{fr.50\%}$ = 380 MPa[18]
ESD [J]	0.16 (nano-K-6, 75 nm particle size)[8], 0.09 (2.0 J @ 500 Ω)[14], 1.0 (K-6/Viton A, 95:5)[14]

https://doi.org/10.1515/9783110672565-010

N [%]	35.60
$\Omega(CO_2)$ [%]	–6.78
$T_{m.p.}$ [°C]	184–185 (dec.)[2], 177–179 (crude K-6)[14], 184–185 (crystals)[14], 180–181 (crude)[14], 180–182 (recryst. from CH_3CN)[14], no melting – gas bubble interacts with (s) phase and forms (l) phase[15], 180–181 (single recryst. from acetone)[16], no endothermic process (melting) observed (DTA, various conditions)[17]
$T_{sublimation}$ [°C]	No endothermic process (sublimation) observed (DTA, various conditions)[17]
$T_{dec.}$ [°C]	184–185 (dec.)[2], 173 (exo, onset), 181 (exo, peak max) (DSC @ 2 °C/min, 26 mg sample)[2], 144.1 (onset, hydrolysis), 168.2 (exo, onset) (TG @ 2 °C/min, 26 mg sample)[2], 189.57 (peak max, DSC @ 10 °C/min, nano-K-6)[5], 186.17 (peak max, DSC @ 5 °C/min, nano-K-6)[5], 193.47 (peak max, DSC @ 15 °C/min, nano-K-6)[5], 196.37 (peak max, DSC @ 20 °C/min, nano-K-6)[5], 196.73 (peak max, DSC @ 10 °C/min, micro-K-6)[5], 155 (onset of mass loss, TG, nano-K-6)[5], 165 (onset of mass loss, micro-K-6)[5], 187 (DTA, nano-K-6)[5], 195 (DTA, micro-K-6)[5], 205 (exo, DSC)[6], 188 (onset, exotherm), 195 (exotherm peak max) (DSC @ 5 °C/min)[9], 211.4 (exotherm, peak max, DSC @ 10 °C/min, 0.1 MPa, 98.5% purity of K-6)[13], two stage thermal dec. process: 189.61 °C and 213.78 °C (TG-DTG, ~ 21.45% mass loss in first stage, 77.83% mass loss in second stage, 98.5% purity of K-6)[13], 204.9 (DSC)[14], 203.0 (DSC, K-6/Viton A, 95:5)[14], 188 (onset, exo), 195 (exo peak max) (DSC @ 5 °C/min)[15]

TG-DTA @ 10 °C/min of K-6 and PBXs (K-6 V 9505 = 95% K-6, 5% Viton A; K-6 V 9010 = 90% K-6, 10% Viton A; K-6 K 9505 = 95% K-5, 5% Kel-F; K-6 K 9010 = 90% K-6, 10% Kel-F), T_i = onset T, T_s = inflection T, T_f endset T[17]:

Sample	TG				DTA	
	T_i (°C)	T_s (°C)	T_f (°C)	% mass loss	Exo peak T (°C)	Integral normalized peak area ($°C^2\,mg^{-1}$)
K-6	191	199	203	89.6	202	183.2
K-6 V 9505	186	193	197	87.9	195	229.2
	434	440	449	1.5	–	–
	464	477	486	3.7	483	450.0
K-6 V 9010	185	194	195	83.2	193	214.5
	438	443	450	2.0	–	–
	470	483	492	7.8	488	397.6
K-6 K 9505	187	194	197	87.8	196	280.8
	426	441	448	5.7	–	–
K-6 K 9010	186	193	196	79.6	194	133.6
	413	418	426	3.6	–	–
	439	445	451	6.8	–	–

TG-DTA @ 10 °C/min of K-6 and PBXs in air atmosphere (K-6 V 9505 = 95% K-6, 5% Viton A; K-6 V 9010 = 90% K-6, 10% Viton A; K-6 K 9505 = 95% K-5, 5% Kel-F; K-6 K 9010 = 90% K-6, 10% Kel-F), SDT = starting dec. T, FDT = final dec. T[17]:

Sample	TG (static air)			DTA (flowing air) Exo peak *T* (°C)
	SDT (°C)	FDT (°C)	% of dec.	
K-6	184	201	89.0	193
Vacuum	–	–	–	192
Sealed	–	–	–	196
K-6 V 9505	181	195	88.0	188
K-6 V 9010	180	192	81.7	186
K-6 K 9505	182	196	87.9	189
K-6 K 9010	179	195	82.0	186

ρ [g cm^{-3}]	1.932[2, 3, 6], 1.93[5], 1.932 (crystal)[14], 1.930[20]		
Heat of formation	−44.0 kcal/kg (enthalpy of form.)[1], −41.8 kJ/mol ($\Delta H_f°$)[3, 19], −41.9 ± 4.2 kJ/mol[5], −45.46 kJ/mol (ΔH_f (s), calcd.)[7], −10 ± 1.0 kcal/mol (using exptl. heat of combustion)[14], −58.0 kJ/mol (condensed phase enthalpy of form., calcd., EDPHT 2.0)[19], −57.9 kJ/mol (condensed phase enthalpy of form., calcd., S-D method)[19], −182 kJ/kg ($\Delta H_f°$)[20]		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]		1,256 kcal/kg (@ 1.587 g cm^{-3}, calcd.) [H_2O vapor][1] Q_{cal} = 5543 kJ/kg[20]	1,325 kcal/kg (@ 1.587 g cm^{-3}) [H_2O vapor][1]
T_{ex} [K]		3,887 (@ 1.932 g cm^{-3}, ΔH_f = −41.9 kJ/mol, calcd., JAGUAR)[10]	
$p_{C\text{-}J}$ [kbar]		36.45 GPa (@ 1.86 g cm^{-3}, calcd., K-J)[7] 37.98 GPa (@ 1.93 g cm^{-3}, calcd., K-J)[7] 36.4 GPa (@ 1.932 g cm^{-3}, ΔH_f = −41.9 kJ/mol, calcd., JAGUAR)[10]	379.8 (@ 1.857 g cm^{-3}, K-6/Viton, 95:5)[14]

		396.8 (@ 1.898 g cm^{-3}; 98.5% TMD, K-6/Viton, 95:5, est. value)[14] 409 (@ 1.927 g cm^{-3}; 100% TMD, K-6/Viton, 95:5, est. value)[14] 36.0 GPa (@ 1.930 g cm^{-3})[20]	
VoD [m s^{-1}]		>9,000[2] 8,970 (@ 1.86 g cm^{-3}, calcd., K-J)[7] 8,814 (@ 1.93 g cm^{-3}, calcd., K-J)[7] 9,280 (@ 1.932 g cm^{-3}, $\Delta H_f = -41.9$ kJ/mol, calcd., JAGUAR)[10] 8,690 (@ 1.86 g cm^{-3}, K-6/Viton, calcd., JAGUAR)[10] 8,958 (@ 1.898 g cm^{-3}, 98.5% TMD, K-6/Viton, 95:5, est. value)[14] 9,059 (@ 1.927 g cm^{-3}, 100% TMD, K-6/Viton, 95:5, est. value)[14] 9,170 (@ 1.930 g cm^{-3}, calcd.)[20]	8,810 (@ 1.86 g cm^{-3}, K-6/Viton, 95:5)[10] 8,814 (@ 1.857 g cm^{-3}, K-6/Viton, 95:5)[14]
V_0 [L kg^{-1}]			

LSGT [cm]	$P_{cr} = 2.0$ GPa (critical pressure of detonation initiation, calcd., LSGT)[20]
5 s explosion T [°C]	170 (Wood's metal bath)[9, 15]
Ignition T [°C]	Ignition delay (t_{id}) and activation energy for thermal ignition (E*) and correlation coefficient (r) for K-6 and PBXs measured using tube furnace technique[17]:

Sample	t_{id} (s) at T (°C)				
	200	250	300	350	500
K-6	79.85	39.25	28.88	20.55	13.12
K-6 V 9505	111.78	56.45	42.42	24.63	15.30
K-6 V 9010	106.72	48.30	39.44	27.50	15.10
K-6 K 9505	111.00	47.40	43.38	26.64	12.44
K-6 K 9010	111.45	49.75	33.32	28.47	13.70

Thermal stability

Total mass loss over 155–190 °C range = 92% (micro-K-6, TG-DTA)[5], thermal stability of nano-K-6 is lower than that of micro-K-6[5], unstable >130 °C and will self-heat to a self-sustained dec. if maintained at this temperature[15]

Microcalorimetry @ 65 °C shows higher reactivity of K-6 cf. RDX[15]:

Heat production (μW)	Time (days)	Heat production (μW)	Time (days)
44	1	16	20
44	5	11	25
30	10	10	30
22	15		

Rate constants and Arrhenius parameters for dec. of K-6 in different solvents (sample 1 = K-6 prepared by slow cooling of recryst. soln., 2 mm grain size results; sample 2 = fast crystallization, 0.035 mm grain size results)[16]:

Medium	$10^{-6}k$ (s^{-1}) at various T						E (kcal/mol)	log$A$ [s^{-1}]
	100 °C	110 °C	120 °C	130 °C	140 °C	150 °C		
Benzene	–	1.4	4.5	15	44	125	36.2	14.80
Diphenyl	–	–	4.1	–	38	–	35.9	14.58
o-Dichloro-benzene	–	–	2.0	7.2	22	62	36.5	14.65
Triacetin	–	–	7.7	22	61	162	33.4	13.46
Cumene	–	–	–	–	73	–	–	–
1,5-Dimethyl-naphthalene	–		–	–	71	–	–	–
Sample 1	0.012	0.044	–	0.44	1.28	–	35.4	12.84
Sample 2	–	–	–	–	1.87	–	–	–

Stability of K-6 @ 80 °C is two orders of magnitude lower than that of RDX[16]

<table>
<tr><td>Burn rate [mm/s]</td><td>Burn rate characteristics: pressure interval = 0.1–10.1 MPa, pressure exponent = 0.961, burning rate @ 10 MPa = 55.6 mm/s, strand ρ = 1.74 g cm^{-3}, adiabatic flame T @ 10 MPa = 3419 K[3]</td></tr>
<tr><td>Solubility [g/mL]</td><td>Can be recryst. from ethyl acetate and CH_3CN[2], recryst. from CH_3CN[14], soluble in acetone (NMR)[14], recryst. from ethyl acetate[15]</td></tr>
<tr><td>Hygroscopicity</td><td>Hydrolysis begins @ 25 °C[2]</td></tr>
<tr><td>Compatibility</td><td>Sensitivity of Keto-RDX to hydrolysis[2]:

<table>
<tr><td>Condition of hydrolysis</td><td>Mass decrement (%)/time</td><td>Mass decrement (%)/time</td></tr>
<tr><td>H_2O, 25 °C</td><td>4 %/4 days</td><td>11%/11 days</td></tr>
<tr><td>H_2O, 50 °C</td><td>6%/3 h</td><td>17%/10 h*</td></tr>
<tr><td>H_2O, 100 °C</td><td>Complete dec. in 30 min</td><td></td></tr>
<tr><td>1% aq. HNO_3, 50 °C</td><td>7 %/3 h</td><td></td></tr>
<tr><td>1% aq. NaOH, 50 °C</td><td>7%/3 h</td><td></td></tr>
</table>
*Reaction with fresh H_2O

After stirring in 2:1 (v/v) mixture of acetic anhydride and 90% fuming nitric acid @ –10 °C for 5 min and subsequently warming the mixture up to RT for 16 h K-6 was recovered in 98%[14], stirring K-6 in water with 16% nitric acid and 16% acetic acid @ RT for 15 h and subsequent cooling to 4 °C allowed 77% recovery of the K-6[14]</td></tr>
<tr><td>Activation energy to dec. [kJ/mol]</td><td>36.2 (in benzene)[5], 35.4 (solid state)[5]</td></tr>
<tr><td>Heat capacity [J mol^{-1}]</td><td>110.15 @ 200 K, 147.97 @ 298 K, 148.65 @ 200 K, 180.72 @ 400 K, 203.98 @ 500 K, 220.85 @ 600 K, 230.42 @ 700 K, 235.32 @ 800 K (standard molar heat capacities, calcd.)[7]</td></tr>
<tr><td>Laser ignition</td><td>K-6 laser det. shots with a 1,000 µm diameter spot size, 0.1% HGN dopant level, doped K-6 pressed into a brass body into a 5 mm diameter, 3 mm long cavity @ ~ 75% bulk density with fused silica window (0.4 mm thick) that is AR coated for 810 nm laser diode[11]:

<table>
<tr><td>Laser det.</td><td>Power (w)</td><td>Material</td><td>Function t</td><td>Energy (mJ)</td><td>Spot (mm)</td></tr>
<tr><td>10</td><td>10.8</td><td>K-6</td><td>17.08 ms</td><td>184.46</td><td>1.00</td></tr>
<tr><td>14</td><td>10.8</td><td>K-6</td><td>24.56 ms</td><td>265.26</td><td>1.00</td></tr>
<tr><td>16</td><td>10.8</td><td>K-6</td><td>19.03 ms</td><td>205.52</td><td>1.00</td></tr>
<tr><td>18</td><td>10.8</td><td>K-6</td><td>24.07 ms</td><td>259.96</td><td>1.00</td></tr>
<tr><td>13</td><td>10.8</td><td>K-6</td><td>24.17 ms</td><td>261.04</td><td>1.00</td></tr>
<tr><td></td><td></td><td>Mean</td><td>21.78 ms</td><td>235.25</td><td></td></tr>
<tr><td></td><td></td><td>Std. dev.</td><td>3.11 ms</td><td>33.58</td><td></td></tr>
</table></td></tr>
</table>

<table>
<tr>
<td></td>
<td>K-6 laser det. shots with a 800 μ diameter spot size, 0.1% HGN dopant level, doped K-6 pressed into a brass body into a 5 mm diameter, 3 mm long cavity @ ~ 75% bulk density with fused silica window (0.4 mm thick), that is AR coated for 810 nm laser diode, all with 10.8 W laser power and 0.80 mm spot size[11]:
<table>
<tr><th>Laser det</th><th>Function t</th><th>Energy (mJ)</th></tr>
<tr><td>28</td><td>12.87 ms</td><td>139.00</td></tr>
<tr><td>12</td><td>16.70 ms</td><td>180.36</td></tr>
<tr><td>1</td><td>15.03 ms</td><td>162.32</td></tr>
<tr><td>2</td><td>17.13 ms</td><td>185.00</td></tr>
<tr><td>20</td><td>13.35 ms</td><td>144.18</td></tr>
<tr><td>21</td><td>15.99 ms</td><td>172.69</td></tr>
<tr><td>22</td><td>16.03 ms</td><td>173.12</td></tr>
<tr><td>17</td><td>13.07 ms</td><td>141.16</td></tr>
<tr><td>29</td><td>14.79 ms</td><td>159.73</td></tr>
<tr><td>25</td><td>14.87 ms</td><td>160.60</td></tr>
<tr><td>27</td><td>14.39 ms</td><td>155.41</td></tr>
<tr><td>3</td><td>14.07 ms</td><td>151.96</td></tr>
<tr><td>7</td><td>14.52 ms</td><td>156.82</td></tr>
<tr><td>24</td><td>12.12 ms</td><td>130.90</td></tr>
<tr><td>6</td><td>15.16 ms</td><td>163.73</td></tr>
<tr><td>8</td><td>15.37 ms</td><td>166.00</td></tr>
<tr><td>28</td><td>12.08 ms</td><td>130.46</td></tr>
<tr><td>31</td><td>12.27 ms</td><td>132.52</td></tr>
<tr><td>Mean</td><td>14.43 ms</td><td>155.89</td></tr>
<tr><td>Std. dev.</td><td>1.50 ms</td><td>16.23</td></tr>
</table>
</td>
</tr>
<tr>
<td>CRT</td>
<td>0.031 cm^3/0.25 g @ 80 °C[14], 0.44 cm^3/0.25 g @ 120 °C[14], 0.049 cm^3/0.25 g @ 80 °C (K-6/Viton A, 95:5)[14], 0.886 cm^3/0.25 g @ 120 °C (K-6/Viton A, 95:5)[14]</td>
</tr>
</table>

	K-6[4]	**Keto-RDX**[13]	**Keto-RDX**[16]
Chemical formula	$C_3H_4N_6O_7$	$C_3H_4N_6O_7$	$C_3H_4N_6O_7$
Molecular weight [g mol^{-1}]	236.113	236.113	236.113
Crystal system		Orthorhombic	
Space group	*Pna*2(1)*	*Pnma*	*Pna*2(1)*
a [Å]	10.030(2)	10.057(17)	10.030(2)
b [Å]	5.970(1)	13.483(2)	5.970(1)
c [Å]	13.445(3)	5.982(10)	13.445(3)
α [°]	90	90	90
β [°]	99.00	90	99.00
γ [°]	90	90	90
V [Å^3]	805.1(3)	811.2(2)	805.1(3)
Z	4	4	4
ρ_{calc} [g cm^{-3}]	1.948(3)	1.933	1.948(3)
T [K]		296	293
	* The *Pna*2_1 space group is orthorhombic, however a *β* angle of 99.0° and not 90° was given in the original paper	Crystals obtained from acetone/H_2O soln. K-6 left standing for 3 days @ RT	* The *Pna*2_1 space group is orthorhombic, however a *β* angle of 99.0° and not 90° was given in the original paper

Nano-K-6 shows the same diffraction angles as micro-K6.[5]

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L

Lead azide

Name [German, acronym]:	Lead azide [Bleiazid, LA][†]
Main (potential) use:	Primary explosive, initiating agent, technical LA used in detonators[20], often used as the main primary explosive in detonators and blasting caps[23], primers and detonators but is usually coated with a layer of sensitizer[33]
Structural formula:	$Pb(N_3)_2$

[†] Technical lead azide (LA): LA precipitated in presence of dextrin, 90–85% purity[20]

Dextrinated LA (DLA):	LA in which dextrin is incorporated desensitizes the LA by preventing the formation of large crystals; most common type of LA used commercially[23, 54], also known as Type I LA in which Dextrin is used as a colloidal agent[8], least sensitive/best for handling, 93% with dextrin crystal modifier (spherical)[45], safest-to-handle form and most commonly used commercially[54], lower performance and more hygroscopic[54], ~92% purity, made by adding 3% NaN_3 soln. made slightly alkaline (using NaOH and also containing potato dextrin approx. 6% of expected LA yield) to an equal volume of 7% lead acetate soln. maintained at 60 °C, over time period of 30 min.[59]
Service LA (SLA):	LA is not coated, acetic acid and sodium carbonate are added to act as nucleating agent to precipitate LA in a spherical morphology which is less hazardous than the highly sensitive needle-shaped LA crystals[23, 54], LA crystals each contain a nucleus of lead carbonate, 96.1% LA[8], has a higher explosive performance than DLA or RD1333/SPLA but is more sensitive[54], phlegmatized LA, equant transparent crystals, made by near simultaneous addition of 1 M lead acetate soln. (added slightly in advance) and 2 M sodium azide soln. to kettle which contains some sodium carbonate soln.; lead carbonate is also produced which acts as a nucleating or seeding agent controlling crystal growth of LA; 96% pure, more energetic than DLA; more sensitive than DLA[59]
Special purpose LA (SPLA):	LA is desensitized by the sodium salt of carboxymethylcellulose (CMC), often used in military applications[23], both forms (SPLA = US developed; RD1333 = British developed) utilize the sodium salt of CMC as the desensitizing agent[54]

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On-demand LA:	LA which meets specifications of SPLA and RD1333, produced in on-demand process, qualified by US Army in 2012 and is currently undergoing evaluation[54]
Colloidal lead azide (CLA):	CLA, also known as Type II LA; non-DLA with very small particle size, 99.9% LA[8], purest form of LA used in the US[54], made by mixing dil. solns. of lead and azide salts[54], very fine particle size (~5 µm) and extremely sensitive to ESD[54], main use is as coating on electric bridge wires for commercial electric detonators[54]; not colloidal in its particle size [59]
Polyvinylalcohol (PVA)-LA:	LA crystals coated with polyvinylalcohol, normal LA content is 93–96%[8], high performance, 96% with polyvinyl alcohol as crystal modifier[45], crystalline form precipitated in presence of PVA; well-defined, transparent crystals, 96% purity, may contain some PVA combined with lead; initiating efficiency equal to SLA and similar sensitivity[59]
RD-1333:	Insensitive form of LA with nonpublished manufacture process, 98.7% LA[8], most sensitive/high performance, 98.7% with CMC added to control the particle characteristics[45]
Dextrinated colloidal: LA (DCLA):	LA with a very small particle size in the range of 1–2 µm, 92.7%–95.3 LA[8]
RD1352:	Spheroidal form of DLA, low dextrin content[59]

(Detailed descriptions of the processes for the preparation of different types of LA can be found in reference[59])

Types of LA used in reference[34]:

	Dextrinated	RD 1333	PVA	Service	British colloidal
LA (%)	92.8	98.7	96.0	98.1	99.9
Particle size average (µm)	24.5	34.5	19.0	55.0	3.4

	LA
Formula	N_6Pb
Molecular mass [g mol^{-1}]	291.3
Appearance at room temperature [RT]	Buff solid (DLA)[8], white solid (SLA)[8], white solid (CLA)[8], white–buff solid (PVA-LA)[8] white–yellowish crystals[15], white solid[20], fine-grained crystalline material[29], pure crystals are colorless[29], DLA is yellow-white[29], LA can vary from white–cream colored–gray[29], white-buff solid[33], white–buff (colloidal LA, 99.0 +% purity, average particle = 5 µm)[60], white–buff (special-purpose LA, RD1333, 98.5% purity, opaque, irregular, no translucent crystals)[60], white – buff (DLA, 91.5% purity, average particle = 70 µm, no needle-shaped crystals)[60]
IS [J]	10 cm (2 kg mass, 20 mg sample, B.M.)[2, 33], 3 in (2 kg mass, 30 mg sample, P.A.)[2, 33], 17 cm (DLA, 2 kg mass, 20 mg sample, B.M.)[2, 33], 5 in (dextrinated, 2 kg mass, 28 mg sample, P.A.)[2, 33], 2.5–4.0[3], 2.5–4 Nm[7, 41], 2 cm (2 kg mass)[5], 30–40 cm (500 g mass)[5], 35–40 cm (2 kg hammer)[5], 43 cm (B.M.)[5], 113 cm (median height, 2 kg mass, 30 mg sample, Rotter apparatus)[6], 0.089 (LA RD1333)[23], 0.089 ± 0.054 (LA RD1333)[23], 3 in (30 mg sample)[36], 75 cm (B.M.)[36], 100 cm (SLA)[39], 100 cm (BLA)[39], <15 kg-cm[40], 2.5–4[55], 24 cm (100% fire, 400 g hammer, 20 mg sample)[56], 10.5 cm (100% no fire, 400 g hammer, 20 mg sample)[56] Powdered samples: $H_{50\%}$ = 4 cm (NOL)[6], $H_{10\%}$ = 17 cm (B.M.)[6], $H_{10\%}$ = 5 in (P.A.)[6] $H_{50\%}$ = 15.24 cm (ball and disc impact test, SLA)[16], $H_{50\%}$ = 15.04 cm (ball and disc impact test, β-LA)[16], $H_{50\%}$ = 7.35 cm (ball and disc impact test, α-LA)[16], 9 cm (2 kg mass)[20] Sensitivities of mechanical mixes of different types of LA (ball and disc impact test)[16]: $H_{50\%}$ = 15.24 cm (ball and disc impact test, SLA)[16], $H_{50\%}$ = 11.91 cm (ball and disc impact test, 90% service LA, 10% β-LA)[16], $H_{50\%}$ = 10.31 cm (ball and disc impact test, 90% SLA, 10% γ-LA)[16] Sensitivity of LA increases as particle size increases. Crystals of 1 mm length are liable to spontaneously explode due to internal stresses. US Ordnance Department specifications allow LA to contain no needle-type crystals which are longer than 0.1 mm[20]. Crystalline SLA becomes more sensitive on storing under H_2O due to an increase in crystal size[20]. LA shows almost the same sensitivity to impact when it is wet as when it is dry[20] Minimum hot spot *T* for initiation by impact = 500–550 °C (in presence of grit)[21], work = 4.76 kg•m•cm^2, drop weight = 975 mg, upper limit = 235 cm, lower limit = 65–70 cm[24]

Values from[8]:

	DLA, type I, US	SLA	CLA, type II, US	PVA-LA, US	RD1333	DCLA
P.A., 2 kg mass	4–6 in	2 in	2–3 in	4–5 in	5 in	3–6 in
Mass of sample (mg)	28	37	25	30	23	18
B.M., 2 kg mass	13–28 cm	30 cm		13–16 cm	15 cm	
P.A., 500 g mass	12 in		6 in	18 in	15 in	
Mass of sample (mg)	28			31	21	
B.M., 500 g mass	100+ cm		35 cm	100+ cm	100+ cm	

All LA dextrinated, IS, 2 kg weight, values given in inches PA apparatus[2]:

LA dry	LA + 25% H_2O	LA + 20% H_2O	LA + 20% ethyl alcohol
4	9	9	4

IS of wet and dry LA (2 kg mass, P.A.)[8]:

Composition (%)			Impact test (in)
LA	H_2O	EtOH	
100	–	–	4
80	20	–	9
80	–	20	4
75	25	–	9

Ball drop IS (steel ball, ball weight = 8.36 g)[34]:

Explosive	$H_{50\%}$ (cm)
Special-purpose LA	56.9 ± 5.3
RD1333 OMC2-2 LA	51.1 ± 8.9
Dextrinated LA 51–127	54.6 ± 8.4

10% point = 7 in (P.A., RD1333 LA, granulation: 1% on 100, 5% on 140, 14% on 200, 42% on 325, 38% through 325)[44], 50% point = 8 in (P.A., RD1333 LA, granulation: 1% on 100, 5% on 140, 14% on 200, 42% on 325, 38% through 325)[44], 10% point = 10 in (ball drop, RD1333 LA, granulation: 1% on 100, 5% on 140, 14% on 200, 42% on 325, 38% through 325)[44], 0.050 ± 0.004 (ball drop, RD1333)[45], 0.089 ± 0.054 (ball drop, RD1333)[45], 21.5 in (50% response, ball drop, 7 g steel ball impacting 0.5 mm thick layer sample, DLA)[47], 5 in (2 kg mass, DLA, P.A.)[47], 20.1 in (50% response, ball drop, 7 g steel ball impacting 0.5 mm thick layer sample, RD1333 LA)[47], 54 ft.lb × 10^{-2} (50% detonation using 50 trials, 9 oz ball, SLA)[53], 69 ft.lb × 10^{-2} (50% detonation using 50 trials, 9 oz ball, DLA)[53], 0.089[54], 10.5 cm (50% explosions, 400 g weight, 20 mg sample)[57]

Ball drop test (8.35 g, ½ in diameter steel ball, 35 mg sample)[49]:

LA	Firing level (%)	Heights (in)					
		Dry	Freon	Freon-10% EtOH	EtOH, 95%	EtOH-H_2O, 50/50	H_2O only
Dextrinated	10	17	8.6	11	≥31	≥31	≥31
	50	20	19	22	≥42	≥42	≥42
RD1333	10	19	7.4	9	11	23	16
	50	26	10	13	14.6	28	37
PVA	10	16	5	7	7	10	11.6
	50	23	9	9	12	21	15
Spec. purp.	10	16	10	11.2	12	10.6	36
	50	22	12	14.4	16	13	40
Average and std. dev.	10	17 (1.5)	8 (2.3)	10 (2.2)	12 (5.5)		21
	50	23 (2.5)	12.5 (3.9)	15 (4.3)	17.5 (5.7)		30

Ball drop impact test (8.35 g, ½ in diameter steel ball, 35 mg sample), height (in)/%[49]:

LA	Dry	Wet with				
		Freon	Freon/10% EtOH	95% EtOH	50% H_2O/50% EtOH	H_2O
Dextrinated	20/50	19/50	24/30	42/50	42/50	42/50
	17/5	9/15	13/10, 13/10	42/10	42/10	42/10
	18/20	10/15	14/15			
		11/15	15/30			
		12/15, 13/25	19/35			
		16/15, 17/30	20/50			
RD1333	26/50	10/50	13/50	20/50	28/50	38/50
	17/10	6/5	8/10	10/5	22/10	21/25
	19/15	7/5	9/10	11/10	23/10	24/30
	20/10	8/15	10/10	12/35	24/10	26/30
	21/15	9,725	11/20	13,730	25/25	29/25, 30/30
PVA	23/50	11/50	12/50	18/50	21/50	25/50, 15/50
	15/10	5/10	6/5	7/10	10/20	10/5
	16/10, 16/10	6/5	7/5, 7/10	8/15	11/15	11/5
	17/5	7/30	8/10	9/25	12/15	12/15
	18/25	8/45, 9/50	9/35	10/20, 13/30, 14/55	13/25, 15/20, 16/25	13/25
Special purpose	22/50	12/50	17/50	16/50	13/50	40/50
	16/15	9/5	9/20	10/5	10/10	35/5
	17/10	10/5	10/10	11/15	11/10, 11/15	36/15
	18/25	11/15	14/50	13/15	12/25, 12/25	38/20
	19/20	12/40	15/45	14/15, 15/30		

Properties of spheroidal and conventional DLA[59]:

Property	Batch no. or product						
	1	2	3	4	5	DUP	KNK
Purity (%)	92.90	93.16	94.43	91.98	93.44	91.50	
Moisture (%)	0.46	0.61	0.57	0.66	0.74		
Bulk ρ (g/mL)	2.15	2.17	2.21	2.12	2.27	1.86	
IS:							
Ball drop (8.3 g/in)	37	39	32	34	29	32	40
Impact (2 kg/in)	7	5	5	4	5	7	

DUP = abbreviation for DuPont DLA; KNK = abbreviation for Kankakee Ordnance Works, USA.

113 cm (2 kg mass, median height, FoI = 20 (cf. lead 2,4-DNR = 11 (standard)), Rotter apparatus)[61]

IS of LA as a function of weight and height (PA apparatus, 20 samples per data point), approx. values taken from graph[61]: $H_{5\%}$ = 3 in (2.0 kg mass)[61], $H_{25\%}$ = 6 in (2.0 kg mass)[61], $H_{60\%}$ = 9 in (2 kg mass)[61], $H_{75\%}$ = 9 in (2 kg mass)[61], $H_{100\%}$ = 15 in (2 kg mass)[61], $H_{25\%}$ = 6 in (3 kg mass)[61], $H_{55\%}$ = 6 in (3 kg mass)[61], $H_{60\%}$ = 6 in (3 kg mass)[61], $H_{20\%}$ = 12 in (1 kg mass)[61], $H_{30\%}$ = 12 in (1 kg mass)[61], $H_{35\%}$ = 15 in (1 kg mass)[61], $H_{50\%}$ = 15 in (1 kg mass)[61], $H_{65\%}$ = 18 in (1 kg mass)[61], $H_{70\%}$ = 21 in (1 kg mass)[61], $H_{85\%}$ = 24 in (1 kg mass)[61], $H_{90\%}$ = 27 in (1 kg mass)[61], $H_{5\%}$ = 18 in (500 g mass)[61], $H_{10\%}$ = 21 in (500 g mass)[61], $H_{35\%}$ = 27 in (500 g mass)[61], $H_{48\%}$ = 30 in (500 g mass)[61], $H_{62\%}$ = 33 in (500 g mass)[61]

Impact initiation delay, delay range for approx. 20 initiations[61]:

Impact energy (J)	Average delay (µs)	Delay range (µs)
6.34	106	40–295
4.85	164	40–380
3.40	296	91–450
1.94	318	50–620
0.98	197	40–810
0.47	114	40–300

Ball and disc IS[61]:

Explosive	Height for 50% reactions (cm)	Standard deviation (cm)
SLA	15.24	0.106
β-LA	15.04	0.078
γ-LA	7.35	0.121
90% SLA/10% β-LA	11.91	0.081
90% SLA/10% γ-LA	10.31	0.149

Effect of T on the IS (2 kg mass, rel. humidity = 60%, 20 samples per data point, Picatinny apparatus) approx. values from graph[61]:

Temperature	% of samples reacting	Height (in)
RT	5	3
RT	15	5
RT	25	6
RT	35	7
RT	60	8
RT	75	9
RT	100	12
−100 °C	5	4
−100 °C	25	6
−100 °C	60	8
−100 °C	70	9
−100 °C	90	11
−100 °C	100	13

% of samples reacting, 2 kg mass, 70°F, rel. humidity = 55%, 20 samples per data point, Picatinny Arsenal apparatus, approx. values from graph[61]:

Height (cm)	LA type				
	SPLA	Colloidal	PVA	RD1333	DLA
5	12	4			
10	60	10		5	0
15	95	25	0	10	10
20	100	60	5	20	50
25		65	15	35	95
30		85	40	75	100
35		95	75	90	
40			100	95	
45				98	

Height (in), ½ in steel ball, 70°F, rel. humidity = 55%, 20 samples per data point, Picatinny Arsenal apparatus, approx. values from graph[61]:

% samples reacting	LA type		
	PVA	RD1333	DLA
0	15	12	13
10	16.5	16.5	16
20	17	20	17.5
30	17.5	22	19
40	18	23.5	20
50	19	24	21
60	19.5	25	22
70	20	25.5	23
80	21	26	24
90	22	27	26

Sensitivity of LA to kinetic energy and impulse, data from[61]

Ball diam (in.)	Bal mass (g)	Height (cm)	*e*	Detonations (%)	Potential energy[a]	Net kinetic energy[b] (J)	Impulse[c] (J •s × 10^{-4})
$^{7}/_{8}$	44.66	90	0.615	10.9 (20)	0.394	0.230	0.310
	44.66	100	0.644	15.0 (20)	0.437	0.256	0.326
	44.66	110	0.613	17.5 (40)	0.482	0.281	0.342
	44.66	120	0.617	20.0 (20)	0.525	0.307	0.358
1	66.68	60	0.510	17.5 (40)	0.392	0.290	0.346
	66.68	80	0.513	35.0 (40)	0.523	0.386	0.403
	66.68	100	0.514	47.5 (78)	0.654	0.483	0.451
	66.68	120	0.509	57.0 (100)	0.784	0.579	0.493
$1^{1}/_{8}$	95.04	100	0.372	80.0 (20)	0.933	0.804	0.580
	95.04	120	0.368	87.5 (40)	1.120	0.965	0.632

[a]Potential energy = mgh; [b]Net kinetic energy = $mg(h_1 - h_2) = 980\ mh_1\ (1 - e^2)$: [c]Impulse or change in momentum = $Ft = m\ (u_1 - u_2) = 44.3$ m$(1 + e)h_1^{1/2}$, where m = ball mass, g = gravitational constant, h_1 = initial fall height, h_2 = rebound height, $e = u_2/u_1 = (h_2/h_1)^{1/2}$ = coefficient of restitution, F = force, t = time over which ball goes from u_1 to u_2, u_1 = falling velocity before duration of contact, u_2 = rebounding velocity after duration of contact

Effect of drying and humidity on IS of SPLA (2 kg mass, PA, 20 samples per data point), % of sample reacting @ specified height[61]:
Sample air-dried for 24 h: 15% @ 4 in, 45% @ 5 in, 70% @ 7 in, 75% @ 8 in, 78% @ 10 in, 95% @ 13 in[61]
Sample air-dried for 2 days: 10% @ 1 in, 40% @ 3 in, 70% @ 4 in, 95% @ 4.5 in[61]
Vacuum dried @ 60 °C for 24 h: 5% @ 1 in, 10% @ 2 in, 45% @ 3 in, 75% @ 4 in, 85% @ 5 in[61]
Sample dried in vacuum for 24 h @ 60 °C: 5% @ 3 in, 30% @ 4 in, 75% @ 5 in, 85% @ 7 in, 88% @ 6 in[61]
Sample dried in vacuum for 24 h @ 60 °C then allowed to stand @ 65% RH for 24 h: 15% @ 3 in, 40% @ 4 in, 60% @ 5 in, 68% @ 7 in, 98% @ 10 in[61]

FoI = 18–20 (RD1333 LA, Rotter machine)[61], FoI = 21 (RD1343 LA, Rotter machine)[61]

$H_{10\%}$ (RD1343 LA, PA): 12.7 cm (2 kg mass), 33 cm (1 kg mass), 50.8 cm (0.45 kg mass), 150 cm (0.23 kg mass)[61], $H_{10\%}$ (RD1343 LA, ball drop): 83.8 cm (2 kg mass), 76.2 cm (1 kg mass), 58.4 cm (0.45 kg mass), 55.3 cm (0.23 kg mass)[61]

DLA stored for ~25 years in 50:50 H_2O/EtOH had no significant change in IS[61]

Changes in IS of LA due to storage[61]:

Sample	Storage time (months)							
	As received		6.5		10.5		14.75	
	10%	50%	10%	50%	10%	50%	10%	50%
SPLA								
Lot 1	6.50	8.20	5.10	6.80	5.19	6.95	5.10	6.82
Lot 2	6.77	9.41	4.48	7.20	5.22	7.02	5.05	7.00
Lot 3	6.39	8.66	4.78	7.45	5.13	6.61	7.60	9.70
Lot 4	6.20	9.64	6.20	8.78	5.25	7.25	6.38	7.78
Lot 5	6.29	8.37	4.89	7.61	4.81	6.78	5.27	7.23
Lot 6	3.48	6.72	3.35	5.95	4.58	6.38	5.21	6.53
RD1333								
Lot 1	6.96	8.76	3.02	5.74	4.76	6.44	3.93	6.29
Lot 2	5.12	7.02					5.14	7.62

Effect of liquid nitrogen on the IS[61]:

	DLA	PVA LA	RD1333 LA
A) Mean height for 50% probability of reactions			
Control (dry): height (cm)/σ	32.13/5.05	28.75/3.33	31.75/12.29
LN_2 test: height (cm)/σ	43.31/6.58	33.02/9.32	31.75/5.18
B) Height for 10% probability of reactions*			
Control (dry): height (cm)	15.24† (12.70)	12.70 (7.62)	12.70 (7.62)
LN_2 test: height (cm)	25.4	15.24	12.70
C) Effect of temperature cycling @ 50% height‡			
In LN_2: % fire§	55	35	45
Dry: % fire§	45	50	60

* 2 kg weight in modified PA apparatus for 10% point; † values in () indicate 10% point in regular PA test; ‡ temperature cycling consisted of soaking sample in LN_2 for 15 min and the allowing to stand @ ambient *T* for 1 h for five cycles; 20 samples tested dry and 20 in LN_2; § % fire in cycled tests indicates % samples fired of 20 samples tested at control 50% fire height

Ball drop apparatus, DLA[65]:

Ball diameter (in)	Ball mass (g)	Height (h_1) (cm)	E	Detonations (%)	mhg (ergs × 10^{-6})	Net kinetic energy (ergs × 10^{-6})	impulse (cgs units × 10^{-4})
$^7/_8$	44.66	90	0.645	10.0	3.94	2.30	3.10
$^7/_8$	44.66	100	0.644	15.0	4.37	2.56	3.26
$^7/_8$	44.66	110	0.643	17.5	4.82	2.81	3.42
$^7/_8$	44.66	120	0.647	20.0	5.25	3.07	3.58
1	66.68	60	0.510	17.5	3.92	2.90	3.46
1	66.68	80	0.513	35.0	5.23	3.86	4.03
1	66.68	100	0.514	47.5	6.54	4.83	4.51
1	66.68	120	0.509	57.0	7.84	5.79	4.93
$1–^1/_8$	95.04	100	0.372	70.0	9.33	8.04	5.80
$1–^1/_8$	95.04	120	0.368	87.5	11.20	9.65	6.32

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; RD1343 LA, data from[66]

Rotter impact data		US data	
F of I	Gas evolved (mL)	NSWC/NOL, ERL type 12	NWC B.M. type 12
20	13	12	

Rotter impact data, 20 drop expts., $h_{50\%}$ = median drop height, each drop expt. Has the no. of ignitions out of 20 (n_g), the fraction of ignitions (P_g), average gas volume evolved per ignition (V_g) and calcd. powder explosiveness at each level (X), RD1343 LA, data from[66]

Drop height multiple of $h_{50\%}$	No. of fires out of 20 drops (n_g)	$P_g = n_g/20$	Average gas evolved, V_g (mL)	explosiveness at each level, X (%)
0.67	0	0	0	0
0.75	3	0.15	13.4	100
1.0	8	0.40	13.1	100
1.5	12	0.60	12.9	100
2.0	10/10	1.0	12.0	100

Effect of grit on percussion sensitiveness of LA (% ignitions), weight of ball = 9 oz.[53]:

Impact oz, in	Service azide	Service azide + 9% emery	Dextrin azide	Dextrin azide + 9% emery
31	(2%)	44%	(2%)	10%
40	3%	46%	3%	10%

FS [N]

Explodes with steel shoe (friction pendulum test)[2, 36], explodes with fiber shoe (friction pendulum test)[2], 0.1–1.0[3, 55], 4.46 ft/s (Emery paper test, service LA)[16], 4.39 ft/s (Emery paper test, β-LA)[16], 6.29 ft/s (Emery paper test, α-LA)[16], FoF = 0.84 (rotary friction FoF)[22], FoF = 0.07 (rotary friction FoF)[22], 10 (BAM limiting load)[22], 0.1 (BAM limiting load)[22], <1 (LA RD1333)[23], 0.098 (LA RD1333)[23], E_{50} = 50 g[35], <0.1 kg (BAM)[40], 0.1[41], <1[54], 100% (explosion % of 25 samples under 588.40 kPa and 80° swing angle)[56], 0.02 kgf[57]

Sensitivities of mechanical mixes of different types of LA (Emery paper test)[16]: 4.46 ft/s (SLA)[16], 3.61 ft/s (90% SLA, 10% β-LA)[16], 3.57 ft/s (90% SLA, 10% γ-LA)[16]

Tested on porcelain and Emery paper (Julius-Peters, BAM)[19]:

Type of LA	Friction sensitivity (g)					
	Porcelain	Emery paper grades				
		P80	P100	P120	P180	P360
SLA (service LA)	10	75	20	30	50	50
NA98 (98% LA pure)	20	175	20	30	50	40
NA94 (94% LA phlegmatized)	75	90	50	30	100	200
DLA (dextrinated LA)	100	350	250	75	275	500

Sensitivity of LA increases as particle size increases. Crystals of 1 mm length are liable to spontaneously explode due to internal stresses. US Ordnance Department specifications allows LA to contain no needle-type crystals which are longer than 0.1 mm[20]

Minimum hot spot *T* for initiation by friction = 430–500 °C [21]

F_{50} = 0.26 (dry sample) (FSKM-PEx OZM friction tester, roughened ceramic plate and porcelain peg)[28], F_{50} = 2.47 (5% water) (FSKM-PEx OZM friction tester, roughened ceramic plate and porcelain peg)[28], F_{50} = 8.04 (10% water) (FSKM-PEx OZM friction tester, roughened ceramic plate and porcelain peg)[28], F_{50} = 9.44 (excess water) (FSKM-PEx OZM friction tester, roughened ceramic plate and porcelain peg)[28], 250 g (basic LA)[39], 50 g (SLA)[39]

Friction pendulum test, all samples LA dextrinated[2]:

	LA dry	LA + 25% H_2O		LA + 20% H_2O	
Shoe	Fiber	Fiber	Steel	Fiber	Steel
No. of trials	1	10	12	10	1
Explosions	1	0	0	0	1
Cracklings		0	2	0	0
Unaffected	0	10	10	10	0

FS of wet and dry LA, pendulum friction test[8]:

Composition, %			Pendulum friction test			
LA	H_2O	EtOH	fiber shoe		Steel shoe	
			Trials	Detonation	Trials	Detonation
100	–	–	1	1	–	–
80	20	–	10	0	4	1
80	–	20	1	1	–	–
75	25	–	10	0	12	0

Julius-Peters, BAM, porcelain plate and peg, Bruceton method[34]:

Explosive	Initiation level	
	50% (g)	10% (g)
Colloidal LA	16 ± 7	–
PVA LA	50 ± 22 < 10	
RD1333 OMC2-2 LA	81 ± 29	20
Dextrinated LA 51-127	157 ± 50	100
Dextrinated LA 51-126	167 ± 90	100

Tests performed on same lot of DLA (duPont) which was desiccated for 6 months, Julius-Peters, BAM, porcelain plate and peg, Bruceton method[34]:

Date	50% initiation level (g)
15.10.1980	200.0 ± 022.6
27.10.1980	167.0 ± 088.0
16.01.1981	159.0 ± 045.0
09.03.1981	210.1 ± 147.0
16.03.1981	164.3 ± 048.0
24.04.1981	191.5 ± 052.7

A comparison of friction data at 10% probability of initiation[34]:

	10% probability of initiation	
	Previous work in 6 trials (g)	Present work in 10 trials (g)
LA	10	20

No fire @ 0 g but low fire @ 10 g (small BAM, RD1333)[45]

Samples mixed with 25% glass, 2 oz weight, Bruceton method, test of 25 charges of samples, $\bar{X}$ = height (in) which a 2 oz ball must be dropped to cause the firing of the sample in 50% of the tests[52]:

Explosive	$\bar{X}$ (in)
Dextrinated LA	8.80
RD1333 LA	2.08

Explodes in Picatinny Arsenal test[61]

% ignitions in mallet FS data from[61]

Explosive	Standard wood mallet on anvils of		
	York stone	Hardwood	Softwood
RD1333	100	100	100
Dextrinated LA	100	100	100
SLA	100	100	100
RD1343	100	100	100

Pendulum FS[61]:

Explosive	Fiber shoe	Steel shoe
LA	Failed	Failed
Dextrinated LA	Failed	Failed

Emery paper FS[61]:

Ignitions/trial at strike velocity (ft/s)	Explosive			
	SLA	RD1333	RD1343	Dextrinated LA
2.5	1/20	1/20	1/20	
3	3/20	2/20	2/20	
4	4/20	5/20	5/20	
5	15/20	8/20	8/20	
6	19/20	17/20	17/20	
8				0/10
9				2/10
10				2/10
11				4/10
Type of ignition	Complete	Complete	Complete	Complete

Emery paper FS, 50% values[61]:

Explosive	Velocity of stroke for 50% reactions (ft/s)	Standard deviation, σ (ft/s)
SLA	4.46	0.184
β-LA	4.39	0.185
γ-LA	6.29	0.194
90% SLA/10% β-LA	3.61	0.206
90% SLA/10% γ-LA	3.57	0.242

Sliding block FS, * = with steel on steel surfaces, substantially the same results were obtained with a dead load of 40 lb instead of 6 lb on the tilting table[61]:

Ignitions/trial at velocity strike (ft/s)	Explosive and surface*			
	SLA		DLA	
	Steel on steel	Emery	Steel on steel	Emery
5	0/10	4/10	0/10	
6	1/10	4/10	0/10	
7	0/10	9/10	0/10	
8	0/10	10/10	0/10	
9	0/10		0/10	0/10
10	0/10		0/10	1/10
11	0/10		0/10	1/10
12	0/10		0/10	5/10
13	0/10		0/10	6/10
14	0/10		0/10	10/10

Effects of liquids on sliding block FS, ignitions/trial at 6 lb load, number of ignitions at 14 ft/s; Perminal = sodium salt of isopropyl naphthalene sulfonic acid[61]:

Desensitizer	SLA
Without desensitizer	10/10
Sprayed 20 s w/water or 2/20% glycerin soln.	6/10
Same, plus 0.1% perminal	8/10
Same, plus 0.1% turkey red oil	5/10
One drop EtOH	1/10
20 s spray butyl alcohol	6/10
One drop butyl alcohol	0/10

BAM FS[61]:

Explosive	Reaction observed	Load on porcelain peg (g)	
		10	20
LA	No reaction	2	0
LA	Ignition	0	0
LA	Detonation	4	6

Friction initiation of LA in the presence of grit, height of fall = 60 cm, amount of sample = 25 mg with or without grit[61]:

Grit	Hardness (Moh's scale)	mpt. (°C)	Explosive efficiency (%)
Nil			0
Silver nitrate	2–3	212	0
Silver bromide	2–3	434	0
Lead chloride	2–3	501	30
Silver iodide	2–3	550	100
Borax	3–4	560	100
Bismuthinite	2–2.5	685	100
Glass	7	800	
Chalococite	3–3.5	1,100	100
Galena	2.5–2.7	1,114	100
Calite	3	1,339	100

FS test using Yamada friction apparatus[61]:

Explosive	Particle size (mm)	Additive	Load for 50% ignitions (kg)		
			Emery	Ebonite	Copper
SLA	0.1 – ~0.3	–	1.7	66.0	MOO
		Ground glass 100 mesh	1.2	11.0	8.0

ESD [J]

0.0070[2], 5.0 mJ (LA RD1333)[23], 6.75 µJ (LA RD1333)[23], 0.01 (max. static discharge @ which no ignition occurs)[8], 0.007 (unconfined)[36], 0.007 (confined)[36], 0.0008 (spark insensitivity, basic LA)[39], <3 kv (Sandia standard man model tester)[40], 4.7 mJ[41], 6.75 µJ (LEESA, RD1333)[45], 0.003 (minimum energy, DLA)[47],0.0025 (minimum energy, RD1333 LA)[47], 50,000 ergs (point of 50% fires, fixed-gap method, 0.005–0.010 in gap)[52], 20 ergs (contact discharge, approaching electrode method)[52], 150,000 ergs (RD-1333 LA @ 0.005 in, fixed-gap method)[52], 0.6 ergs (RD1333 LA, contact discharge, approaching electrode method)[52], 5.0 mJ[54], <5 mJ[55], 0.003[56, 57], 0.007 (unconfined)[61], 0.007 (confined)[61], 5.5×10^{-4} (RD1333 LA, parallel plane, fixed gap, spark discharge)[62], 27×10^{-4} (RD1333 LA, approaching needle, spark discharge)[62]

Contact electrostatic discharge sensitivity[52]:

Explosive	Fires
Dextrinated LA	0/5 at 7,000 V, 300 MMF
	1/5 at 8,000 V, 300 MMF
RD1333 LA	1/5 at 20 V, 300 MMF
	4/5 at 50 V, 300 MMF
	5/5 at 100 V, 300 MMF

Discharge between two metallic electrodes, or one metallic electrode and the lower electrode is covered by a piece of conducting rubber[16]:

Value	Service LA	β-LA	α-LA
ESD (M/M needle 250–500 μμF)	20 ergs	12 ergs	11 ergs
R/M minimum capacitance	~400 μμF	~400 μμF	~400 μμF
Minimum energy	2,250 ergs @ 1,500 μμF	2,500 ergs @ 1,000 μμF	3,000 ergs @ 1,000 μμF

Highest ESD energy @ 5,000 V for zero ignition probability[7]:

Highest energy for zero ignition probability		Type of ignition	
Unconfined	Confined	Unconfined	Confined
0.0070	0.0070	deton.	deton.

50 mJ (zero ignition probability, uncoated LA)[35], 32 mJ (zero ignition probability, PVP coated LA)[35]

Ignition values[35]:

Explosive	Capacitance (MF)	Voltage (kV)	Energy (J)	*T* (°C)	RH (%)	remarks
LA (PVP coated)	0.001	10.0	0.050	26.3	53	ignited
LA (PVP coated 97%)	0.01	6.8	0.231	26.1	57	ignited
LA (uncoated)	0.001	11.0	0.0605	26.1	57	ignited

Threshold ignition energies (energy value given is the energy (erg) stored on the capacitor, the energy dissipated in the gap is about one-tenth of this) data from[36]:

Material	Metal/metal electrodes (no added circuit resistance)		Rubber/metal electrodes (10^5 ohm series resistance)	
	Contact sparks, 500 pF	Gaseous sparks, 1,000 pF	Minimum energy	Minimum capacity, pF
LA	20	10,000	2,250	500

0.005 (P.A., RD1333 LA, granulation: 1% on 100, 5% on 140, 14% on 200, 42% on 325, 38% through 325)[44]

Reproducibility of determinations using RD1333 LA (minimum fire point) approaching-electrode electrostatic sensitivity apparatus, 25 trials were carried out at each test level[50]:

Needle plane	2 expts., 2 months apart (oscillatory discharge, series resistance = 0, storage capacitance = 1,176 pF) 1st expt.: 45,000 ergs 2nd expt.: 45,000 ergs
Needle plane	4 expts., 2 weeks between the first and second, one day between second and third, and eight months between the third and fourth (spark discharge: series resistance = 100 kΩ; storage capacitance = 624 pF) 1st expt.: 7,300 ergs 2nd expt.: 5,800 ergs 3rd expt.: 5,800 ergs 4th expt.: 5,800 ergs
Plane–plane	2 expts., three weeks apart (oscillatory discharge, series resistance = 0, storage capacitance = 1,176 pF) 1st expt.: 45,000 ergs 2nd expt.: 45,000 ergs

Effect of spark starting position on results for RD1333 LA (R = 100 kΩ, C = 1,176 pF), approaching-electrode electrostatic sensitivity apparatus[50]:

Base electrode material	Preset gap (mm)	Spark starting position with respect to sample	Energy ($J \times 10^{-3}$)
Steel	0.18	External	3.4
Steel	0.18	Within	2.8
Steel	0.63	External	3.6
Steel	0.63	Within	2.6
Stainless steel	0.18	External	4.2
Stainless steel	0.18	Within	3.3

Approaching electrode electrostatic sensitivity apparatus, RD1333 LA[50]:

Discharge	Minimum energy (10^{-7} J)		
	Approaching needle	Approaching (pin) plane to plane	Fixed gap, parallel plate
Oscillatory	47,000	47,000	3,000
Arc	20,000	19,000	1,700
Spark	4,700	4,500	1,400
	50% point		
Spark	27,000	–	5,500

ESD of spheroidal and conventional DLA[59]:

Property	Batch no. or product					
	1	2	3	4	5	DUP
Purity (%)	92.90	93.16	94.43	91.98	93.44	91.50
Moisture (%)	0.46	0.61	0.57	0.66	0.74	
Bulk ρ (g/mL)	2.15	2.17	2.21	2.12	2.27	1.86
Electrostatic sensitivity (J)	0.0032	0.0058	0.0053	0.0044	0.009	0.0096

DUP = abbreviation for DuPont dextrinated LA; KNK = abbreviation for Kankakee Ordnance Works, USA.

Effect of process parameters on LA[59]:

Batch	CMC	Agitator (rpm)	T (°C)	Bulk ρ (g/mL)	ESD (J)
RD1333	MN83	200	25	1.33	0.0102
		300		1.49	0.0090
				1.49	0.0078
		350		1.46	0.0096
		125		1.01	0.0360
	7MSP	300		1.14	0.0048
	B50			1.48	0.0040
	4MP			2.11	0.0040

	B50			1.53	0.0029
	4M6F			2.02	0.0048
	4M6			2.04	0.0044
	B50			1.89	0.0044
	4NO		37/38	1.40	0.0053
	4M6F		25	2.05	0.0023
			20	2.00	0.0026
			30	2.13	0.0026
			40	1.88	0.0016
			35	1.90	0.0013
		200		1.88	0.0036
		100		1.11	0.0282
		350		2.13	0.0014
		300	25	1.95	0.0036
				2.09	0.0058
				0.85	0.0346
				1.77	0.0063
				2.09	0.0032
				1.81	0.0032
				1.05	0.0063
RD 1343	MN83	250		1.46	0.0038
				1.85	0.0040
	7MSP			1.11	0.0048
	4MP			1.27	0.0032
DuPont RD1333				1.49	0.0040
Special purpose				1.46	0.0063

Comparison of minimum initiation energy of LA with needle-plane and parallel-plate electrodes, RD1333 LA, constant capacitance of 330 pF used, [b]self-commutated by krypton switch[62]:

Series resistance (12)	RC time constant (m/s)	Energy in spark gap (J)	
		Needle plane	Parallel plate
1.5×10^{-1}	*b*	1.3×10^{-3}	3.3×10^{-4}
8.2×10^{1}	2.7×10^{-5}	$> 5.9 \times 10^{-4}$	3.1×10^{-4}
1.0×10^{5}	3.3×10^{-2}	$> 3.1 \times 10^{-4}$	3.1×10^{-4}
6.8×10^{5}	2.2×10^{-1}	2.2×10^{-4}	1.8×10^{-4}
1.2×10^{6}	4.0×10^{-1}	2.0×10^{-4}	1.1×10^{-4}

Comparison of 50% initiation values of RD1333 obtained for the spark starting within or external to the powder ($R = 100$ kΩ, $C = 1{,}176$ pF)[62]:

Base electrode material	Preset gap (mm)	Spark starting position	Energy (J × 10^{-3})
Steel	0.18	External	3.4
Steel	0.18	Within	2.8
Steel	0.63	External	3.6
Steel	0.63	Within	2.6
Stainless steel	0.18	External	4.2
Stainless steel	0.18	Within	3.3

(See additional values at end of section)

N [%]	28.8
Ω [%]	−5.5
$T_{m.p.}$ [°C]	Dec.[2, 36], detonates before melting[29], does not melt but undergoes dec.[30, 33]
$T_{phase\ transition}$ [°C]	160 ($\alpha \rightarrow \beta$, irreversible)[15, 16] ($\Delta H = 0.30 \pm 0.05$ kcal mol^{-1}, crystalline state)[16]
$T_{dec.}$ [°C]	585 K (DSC @ 0.33 K s^{-1}, covered Al pan, Ar atmosphere @ 168 kPa, 0.2–1.0 mg sample, β-LA; $E_a = 110 \pm 6$ kcal mol^{-1} (Rogers and Morris method); E_a for α-LA = 30 kcal mol^{-1} (Kissinger method), 47.7 kcal mol^{-1} (Gomm))[17], 315 (DSC)[23, 54], 320 (DSC, onset, LA RD1333)[23], 240–250[30], 350 (basic LA)[39], 325 (SLA)[39], 315 (exo max, DSC)[41], 332 (onset), 341 (peak) (DSC @ 20 °C/min, RD1333)[45], 315[55], 463 K (onset), 618 (peak max)[57], 317 (DTA-TGA, DLA)[58]

T of DTA exotherms for RD1333 LA (heating rate = 10 °C/min in He)[63]:

T_{onset} (°C)	T_{peak} (°C)	Lead MP (°C)	Sample weight (mg)
287	305	317	2.4
289	305	316	2.6
288	305	320	1.1
293	305	320	1.0
294	306	321	0.8
290	304	320	0.4
288	304	320	0.4
290	304	316	0.4
287	302	316	0.5
290	303	320	0.3
287	302	320	0.3

DTA data, [a]sample detonated, from[63]:

Azide	Heating rate (°C/min)	Exotherm onset (°C)	Exotherm peak (°C)	Δ°C
PVA	5	285	303[a]	18
DLA	5	290	296	6
RD1333	5	288	306	18
	5	297	308	11
PVA	10	296	312	16
DLA	10	298	306	8
RD1333	10	296	312	16
	10	301	317	16
high purity	10	287	302	15
PVA	20	298	316	18
DLA	20	302	314	12
RD1333	20	308	323	15
	20	320	320	10

ρ [g cm^{-3}]

4.80 (crystal)[2, 36], 4.38 (dextrinated)[2], 4.8[4, 23], ~4.8 (true ρ)[20], ~1.2 (apparent ρ of loose powder)[20], 2.58 (LA RD1333)[23], 4.71 (orthorhombic, α-form)[30], 4.93 (monoclinic, β-form)[30], 1.83 (apparent density, DLA type I)[8], 0.85 (apparent density, CLA type II US)[8], 4.7 (crystal)[41], 4.80[54, 55], 4.38[57]

Loading ρ (sample 1)[6, 36]:

Pressure (kpsi)	Loading ρ (g cm^{-3})
3	2.46[6, 36]
5	2.69[6, 36]
10	2.98[6, 36]
12	3.05[6, 36]
15	3.16[6, 36]
20	3.28[6, 36]
Crystal	4.68[6, 36]

Loading ρ (sample 2)[2, 6, 36]:

Pressure (kpsi)	Loading ρ (g cm^{-3})[2, 6, 36]
3	2.62[2, 6, 36]
5	2.71[2, 6, 36]
10	2.96[2, 6, 36]
15	3.07[2, 6, 36]

3.14 (@ 15,000 psi, DLA, type I, US)[8], 3.31 (@ 15,000 psi, SLA)[8], 3.81 (@ 15,000 psi, PVA-LA, US)[8]

Data from[34]:

Explosive	Crystal density (g/cc)
Colloidal LA	4.8
PVA LA	< 4.8
Special-purpose LA	4.8
Dextrinated LA 51-127	4.4
Dextrinated LA 51-126	4.4

	1.3 (bulk density, RD1333 LA, granulation: 1% on 100, 5% on 140, 14% on 200, 42% on 325, 38% through 325)[44] Bulk densities of spheroidal and conventional DLA[59]: Property / Batch no. or product: 1 / 2 / 3 / 4 / 5 / DUP Purity (%): 92.90 / 93.16 / 94.43 / 91.98 / 93.44 / 91.50 Moisture (%): 0.46 / 0.61 / 0.57 / 0.66 / 0.74 / Bulk ρ (g/mL): 2.15 / 2.17 / 2.21 / 2.12 / 2.27 / 1.86 *DUP = abbreviation for DuPont dextrinated LA*
Heat of formation	Enthalpy of form. = 1,637.7 kJ/kg[4], energy of form. = 1,663.3 kJ/kg[4], −368 cal/g[2], 450.1 kJ/mol ($\Delta_f H_m$)[55], 469 kJ/mol[57], 115.5 kcal/mol (standard enthalpy of form., α-LA, cryst, @ 25 °C)[67], 115.8 kcal/mol (standard enthalpy of form., β-LA, cryst, @ 25 °C)[67]
Heat of combustion	630 kcal/kg[2, 12, 36], 2,635 kJ/kg[57]

	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]	1,575	367 kcal/kg[12] Heat of explosion = 1,610 kJ/kg[57]	367 cal/g[2, 36] 1,638[4] 367 cal/g [H_2O (g)][8] 260 cal/g (@ 4.6 g cm^{-3})[30] 1,450 cal/cm^3 (voidless, volumetric heat of explosion, DLA)[36] 970 cal/cm^3 (pressed @ 10,000 psi, volumetric heat of explosion, DLA)[36] 1,760 cal/cm^3 (voidless, volumetric heat of explosion, pure LA[36] 1,100 cal/cm^3 (pressed @ 10,000 psi, volumetric heat of explosion, pure LA[36]

<table>
<tr><td>T_{ex} [K]</td><td>3,285</td><td>3,400 °C[12]

5,600[57]</td><td>3,420 °C[5]

3,450 °C[5]

3,484 °C[5]

3,420–3,484 °C[8]

3,450 °C (@ 4.6 g cm^{-3})[30]</td></tr>
<tr><td>$p_{C\text{-}J}$ [kbar]</td><td>349</td><td>250 (@ 4.0 g cm^{-3}, calcd.)[6]

360 (@ 4.8 g cm^{-3}, calcd.)[6]

33.8 GPa[55]

16.1 GPa (@ 3.9 g cm^{-3})[57]

Exptl. and theoretical detonation pressures of LA, [a] $P = {}^1/_4 \rho D^2$[64]:
<table>
<tr><th rowspan="2">ρ (g/mL)</th><th rowspan="2">VoD (km/ms)</th><th colspan="2">Peak pressure (kbar)</th></tr>
<tr><th>Measured</th><th>Calcd.[a]</th></tr>
<tr><td>3.25</td><td>4.35</td><td>126</td><td>154</td></tr>
<tr><td>3.60</td><td>4.80</td><td></td><td>207</td></tr>
<tr><td>3.78</td><td>5.00</td><td>156</td><td>236</td></tr>
</table></td><td>33.4 GPa[3]

94,930 kg/cm^2 (@ 3.0 g cm^{-3}, under 1,100 kg/cm^2 press)[5]

94,930 kg/cm^2[8]

317 (voidless, DLA)[36]

158 cal/cm^3 (pressed @ 10,000 psi, DLA)[36]

394 cal/cm^3 (voidless, pure LA)[36]

161 cal/cm^3 (pressed @ 10,000 psi, pure LA)[36]

0.922 Mbar[36]</td></tr>
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<td>Exptl. and theoretical detonation pressures of LA,[a] $P = {}^{1}/_{4}\rho D^{2}$[64]:

<table><tr><th rowspan="2">ρ (g/mL)</th><th rowspan="2">VoD (km/ Ms)</th><th colspan="2">Peak pressure (kbar)</th></tr><tr><th>Measured</th><th>Calcd.[a]</th></tr><tr><td>3.25</td><td>4.35</td><td>126</td><td>154</td></tr><tr><td>3.60</td><td>4.80</td><td></td><td>207</td></tr><tr><td>3.78</td><td>5.00</td><td>156</td><td>236</td></tr></table></td>
</tr>
<tr>
<td>VoD [m s^{-1}]</td>
<td>6,077 (@ 4.8 g cm^{-3}; $\Delta_f H = 450$ kJ mol^{-1})</td>
<td>5,920 (@ 4.80 g/cm^3)[55]

4,630 (@ 3.0 cm^{-3})[57]</td>
<td>4,070 (@ 2.0 g cm^{-3}, pressed)[2, 33]

4,630 (@ 3.0 g cm^{-3}, pressed)[2, 33]

5,180 (@ 4.0 g cm^{-3}, pressed)[2, 33]

5,876.8 (@ 4.80 g cm^{-3})[3]

4,500 (@ 3.8 g cm^{-3}, confined)[4, 5]

5,300 (@ 4.6 g cm^{-3}, confined)[4, 5]

5,400 (@ max. ρ)[5]

5,400 (@ TMD)[8]</td>
</tr>
</table>

			4,500 (@ 3.8 g cm^{-3})[8] 5,300 (@ 4.6 g cm^{-3})[8, 11] 5,100 (@ 4.0 g cm^{-3})[12, 47] 5,393 (calcd. based on sand expt.)[11] 5,300 (@ 4.6 g cm^{-3}, calcd. based on sand expt.)[11] ~8,000 (α-$Pb(N_3)_2$ crystals of cross-section ≥2 mm × 2 mm)[14] ~3,000 (α-$Pb(N_3)_2$ crystals of cross section ~1 mm)[14] 4,500 (@ 3.8 g cm^{-3}, loaded into detonator capsules with 7.7 mm internal diameter, Kast)[20] 17,000 ft/s (@ 4.0 g/mL)[29] 4,500 (@ 3.6 g cm^{-3} (pressed))[30] 5,300 (@ 4.6 g cm^{-3})[30]

5,400 (@ max. pressed ρ)[30]

VoD for LA in different metal holders, samples pressed @ 10,000 psi, ρ of 3.22 g/mL[64]:

Holder material	VoD (km/s)
Steel	4.52 ± 0.25
Aluminum	4.85 ± 0.61
Brass	4.65 ± 0.31

Exptl. and theoretical detonation pressures of LA,[a] $P = {}^{1}/_{4}\rho D^{2}$[64]:

ρ (g/mL)	VoD (km/Ms)	Peak pressure (kbar)	
		measured	Calcd.[a]
3.25	4.35	126	154
3.60	4.80		207
3.78	5.00	156	236

<table>
<tr>
<td></td>
<td></td>
<td></td>
<td>Effect of preheating @ 250 °C in the presence of water vapor on the subsequent VoD of compressed sheets of LA[16]:
<table>
<tr><th>Duration of heating (min)</th><th>VoD (km/s)</th></tr>
<tr><td>0</td><td>~5,500</td></tr>
<tr><td>5</td><td>~2,300</td></tr>
<tr><td>10</td><td>~900</td></tr>
<tr><td>15</td><td>~600</td></tr>
<tr><td>20</td><td>~400</td></tr>
<tr><td>25</td><td>~250</td></tr>
<tr><td>30</td><td>~<100</td></tr>
</table></td>
</tr>
<tr>
<td>V_0 [L kg^{-1}]</td>
<td>252</td>
<td>308[57]</td>
<td>308 cc/g[2, 5, 8, 36]

231[4]

310 (@ 0 °C and 760 mm Hg, @ 4.6 g cm^{-3})[30]</td>
</tr>
</table>

<table>
<tr><td>Critical temperature of explosion [K]</td><td>Critical temperature of thermal explosion (T_c) with respect to the thickness of the planar crystal (h)[18]:
<table><tr><td>T_c (K)</td><td>h (µm)</td><td>T_c (K)</td><td>h (µm)</td></tr><tr><td>~692</td><td>~5</td><td>~672</td><td>~17</td></tr><tr><td>~690</td><td>~6</td><td>~668</td><td>~22</td></tr><tr><td>~678</td><td>~9</td><td>~664</td><td>~34</td></tr></table></td></tr>
<tr><td>Critical pressure of explosion initiation [GPa]</td><td>$P_{ult} = 0.38 \pm 0.03$[25], $P_{cr} = 0.38 \pm 0.03$[26, 27, 51]</td></tr>
<tr><td>Trauzl test [cm^3, % TNT]</td><td>39% TNT[2, 33], 89% LA, 80% MF, 40% TNT (DLA)[8], 115 cc (10 g charge)[6],
16% more net expansion cf. PETN[20], 7.2 cc (1 g LA in no. 8 detonator capsule compressed under a reinforcing cap @ 3,400 lb/in^2 and fired in small Trauzl block)[20]</td></tr>
<tr><td>Sand test [g]</td><td>40% TNT (DLA)[8], 95% pure LA (DLA)[8], 18.6 g sand crushed (1,700 g bomb, 0.4 g LA)[11], 19.0 g (200 g bomb)[33]</td></tr>
<tr><td></td><td>Weight (g) of sand pulverized finer than 30 mesh, no. 8 detonator capsule, pressed under reinforcing caps @ 3,400 lb/in^2, fired in no. 2 sand test bomb[20]:
<table><tr><td>Weight (g) of charge (LA)</td><td>Weight (g) of sand pulverized</td></tr><tr><td>0.10</td><td>3.5</td></tr><tr><td>0.20</td><td>7.2</td></tr><tr><td>0.40</td><td>14.2</td></tr><tr><td>0.60</td><td>21.5</td></tr><tr><td>0.80</td><td>28.7</td></tr><tr><td>1.00</td><td>36.0</td></tr></table></td></tr>
</table>

Initiating efficiency

Initiating efficiency, (g) required to give complete initiation of[2]

HE	Dextrinated azide (g)
TNT	0.25
Tetryl	0.10
RDX	0.05
PETN	0.02

Minimum charge (mg) of LA required to initiate 60 mg RDX in M47 detonator: 90 (DLA, type I, US)[8], 25 (SLA)[8], 100+ (PVA-LA, US)[8], 100+ (RD1333)[8]

Minimum initiating charge (g) of LA required to initiate 0.5 g charge of high explosive (in no. 8 detonator capsule, reinforcing caps, charges compressed under 3,400 lb/in^2)[20]: 0.12 g for PA[20], 0.16 g for TNT[20], 0.03 g for tetryl[20], 0.075 g for trinitroresorcinol[20], 0.05 g for trinitrobenzaldehyde[20], 0.05 g for tetranitroaniline[20], 0.05 g for hexanitrodiphenylamine[20], 0.035 g for pentryl (without reinforcing cap)[20], 0.025 g for tetryl[20], 0.025 g for PA[20], 0.09 g for TNT[20], 0.28 g for trinitroanisole[20]

Minimum charges of LA required for initiating PETN (0.4 g), tamped down or pressed loosely into Cu capsules 6.2 mm inside diameter, primary charge pressed down loosely on top, weights of priming charges decreased until 1 failure in 10 tests occurred, or PETN compressed @ 2,000 kg/cm^2[20]:

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)				
LA (technical)	0.04	0.170	0.05	0.05	0.04
LA (pure)	0.15	0.100	0.01	0.01	0.01

0.025 g (min. charge in no. 8 detonator for tetryl)[41]

Initiating power, minimum amount of primary explosive needed to fully initiate 0.90 grain of high explosive, test piece = brass cup of 0.21 in diameter and 0.70 in long[52]:

High explosive	Dextrinated LA (g)	RD1333 LA (g)
RDX	0.55	0.25
Tetryl	0.35	0.25
HMX	1.05	0.65
PETN	0.35	0.25

Weights of LA required for initiation of secondary explosives[64]:

LA type	Weight (mg)					
	RDX	HMX	Tetryl	Picric acid	PETN	TNT
DLA	90	300	100	260	30	270
SPLA	50					
PVA	25					
SLA	30					

Firing times of hot bridge wire initiators

Sensitivity of LA in wire bridge initiators, W wire 0.030 in long fired @ 14–20 V[36]: 340 Erg for 0.0001 in diameter[36], 1,340 Erg for 0.00029 in diameter[36]

50 mg loads of explosives, voltage of 450 V, times in µs, data from[36]:

Explosive	Milling time (h)	Capacitance, pF		
		0.5	0.05	0.0047
Polyvinyl alcohol LA	24	1.12–1.26	1.09–1.38	1.41–5.00
Dextrinated LA	64	1.08–2.43	1.12–2.43	3.46–4.95

SSGT [cm]

DLA, TMD = 4.71 g/cm^3[43]:

Loading pressure (kpsi)	Density (g/cm^3)		% TMD	Sensitivity (DBG)			
	AVG.	s		AVG.	g	s_m	*N*
4	2.535	0.0280	53.8	−3.622	–	–	18
8	2.775	0.0215	58.9	−0.302	0.3017	0.1839	18
16	3.074	0.0155	65.3	−0.239	0.1672	0.0879	18
32	3.361	0.0215	71.4	−0.227	0.0961	0.0558	18
64	3.663	0.0237	77.8	−0.303	0.3370	0.2120	18

Dead pressing

Not easily dead pressed[33], pressure durability: <118 (or 78) MPa (below this value ICM-103 is dead pressed)[55]

5 s explosion *T* [°C]

330–340 (explodes, US value)[12], 345 (explodes, Russian value)[12], 327 (within 5 s, microcrystalline powder, compressed into pellets weighing 0.02 g)[20], 340 (iron tube)[20], by heating from 315–360 in 5 s[30], 340[2], 340 (DLA, type I, US)[8], 350 (SLA)[8], 344 (CLA, type II, US)[8], 340 (PVA-LA, US)[8], 345 (RD1333)[8], 315–345[8]. 278 (DLA)[8], 340[33, 36], 340 (cook-off)[36], 345[56], 340 (open cup)[61], 340 (DLA, 10 mg sample)[63], 326 (DLA, 20 mg sample)[63], 350 (SLA, 10 mg sample)[63], 358 (SLA, 20 mg sample)[63], 344 (colloidal, 10 mg sample)[63], 340 (PVA, 10 mg sample)[63], 345 (RD1333, 10 mg sample)[63], 340 (unspecified type of LA, 10 mg sample)[63], 342 (20 mg sample, 327 °C = min *T*)[63], 349 (PVA, @ 5 °C/min)[63], 297 (DLA @ 5 °C/min)[63], 335 (RD1333 @ 5 °C/min)[63]

5 s explosion *T* of spheroidal and conventional DLA[59]:

Property	Batch no. or product						
	1	2	3	4	5	DUP	KNK
Purity (%)	92.90	93.16	94.43	91.98	93.44	91.50	
Moisture (%)	0.46	0.61	0.57	0.66	0.74		
Bulk ρ (g/mL)	2.15	2.17	2.21	2.12	2.27	1.86	
Explosion *T* (°C)	301	302	301	299	308	294	301

DUP = abbreviation for DuPont dextrinated LA; KNK = abbreviation for Kankakee Ordnance Works, USA

Explosion *T* [°C]

315 (pure LA)[5], 338 (glass tube @ 20 °C/min)[20], 337 (iron tube @ 20 °C/min)[20], may detonate spontaneously if crystals >1 mm length[33], 383 (instantaneous, pure, dextrinated or RD1333)[52], 315–330 (unspecified type of LA, 300 s ignition delay, 50 mg sample)[63], 340 (unspecified type of LA, 1 s ignition delay, 3 mg sample)[63], >315 (unspecified type of LA, >300 s ignition delay, 3 mg sample)[63]

Sensitization of SLA by preheating, [a]at bath *T*, [b]exploded on withdrawal[63]:

Bath *T* (°C)	Preheat time (s)[a]	Ignition delay (s)
320	0	47
	15	34.8
	25	24.8
	30	24.8
	35	22.8
	43	22.2
	45	0*
330	0	20.3
	5	18.3
	8	16.4
	10	14.6
	15	12.3
	18	11.7
	19	11.3
	20	0[b]

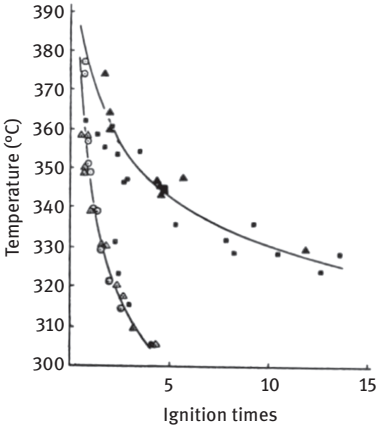
Ignition *T* [°C]

383 (dropped on preheated Wood's alloy)[6], 350[21], 318[48], 600 K[42]

DTA autoignition *T*[34]:

Explosive	Autoignition *T* (K)
Colloidal LA	540
Special-purpose LA	553
RD1333	565
RD1333	557
RD1333	560
Dextrinated LA	557
Dextrinated LA	561

Ignition temperature (Fig. 11) data from[53]



Service azide: ▲ lot 731, ■ lot 606. Dextrin azide: ⊙ lot D. 3, ⊡ lot A. 33, △ lot D. 783.

Fig. 11: Ignition curves of service and dextrin azides[53].

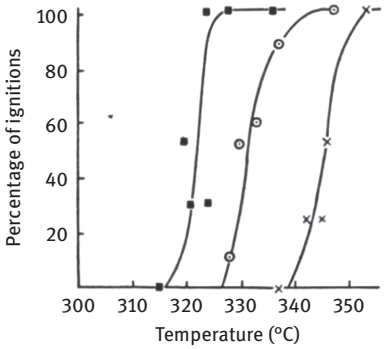
343 (SLA, 5 s delay, extrapolated)[53], 551 (SLA, 10^{-3} s delay, extrapolated)[53], 735 (SLA, 10^{-5} s delay, extrapolated)[53]

Effect of thermal sensitization of LA on subsequent ignition times (service LA, sample heated at a specific temperature for a time insufficient for detonation, sample then rapidly chilled, left to stand for ~1 hour, then heated until detonation resulted at the temperature of the test)[53]:

T (°C)	Preheating time (s)	Subsequent time to ignition of sensitized azide (s)	Total heating time (s)	One stage time to ignition (s)
330	3	4	7	6.6
324	7	–	13	11.5

Percentage ignition, temperature limits for 100 and 0% ignitions[53]:

Initiator	Amount (g)	0% ignitions below (°C)	100% ignition above (°C)
Service azide	0.02	316	326
Dextrin azide	0.01	285	305

Explosion *T* [°C]	Fig. 12 Data from[53]  ■0.02 g. azide; ○ 0.005 g. azide + 0.004 g. glass; × 0.002 g.azide + 0.007 g. glass. **Fig. 12:** Percentage failure-temperature curves for simple initiators[53].
Detonating *T* [°C]	Explosion *T* @ different times of exposure (3 mg samples, detonation)[13]: 0.560 s @ 360[13], 0.865 s @ 341[13], 1.55 s @ 319[13], no action @ 314 °C[13], 335 (12 s)[20], 345 (7 s, iron tube)[20], 350 (4 s, iron tube)[20], 355 (0 s, iron tube)[20], 360 (0 s, iron tube)[20], 396 (0.1 s, no cap used)[2], 356 (1 s)[2, 36], 335 (10 s)[2], 335 (20 s)[2], 396 (0.1 s)[36], >335 (10 s)[36] 335[29], 623 K (deflagration *T*)[35]
Thermal ignition *T* [°C]	335 (calcd.)[36]
Autoignition *T* [°C]	320 (DSC @ 10 °C/min, sealed hermetic cups and lids)[40]
100 °C heat test [% mass loss]	0.34% mass loss in first 48 h[2], 0.05% mass loss in second 48 h[2], no explosion in 100 h[2] Values from[8]:

	DLA, type I, US	SLA	CLA, type II, US	(PVA-LA), US	RD1333
Loss in sample wt.(%) in 8 h		0.11	0.12	0.30	
Loss in sample wt.(%) in 48 h	0.34	0.08		0.13	0.30
loss in sample wt.(%) in 96 h	0.39	0.16			0.30
Explosion in 100 h	None	None		None	None

Vacuum stability test [cm^3/h]

1.0 cc/40 h @ 100 °C (DLA)[2], 0.07 cc/40 h @ 120 °C (DLA)[2], 0.4 cc gas evolved in 40 h @ 100 °C[5]

@ 100 °C gas evolved in mL/g: 0.32 (DLA, type I, US)[8], 0.20 (PVA-LA, US)[8]
@ 120 °C gas evolved in mL/g: 0.46 (DLA, type I, US)[8], 0.44 (PVA-LA, US)[8], 0.43 (RD1333)[8]

0.40 /g @ 150 °C, 40 h (RD1333 LA, granulation: 1% on 100, 5% on 140, 14% on 200, 42% on 325, 38% through 325)[44]

0.07 mL gas evolved after 40 h @ 120 °C[61]

Effect of heat of azides in vacuo[63]:

Azide	*T* (°C)	Weight (g)	Time (h)	Gas evolved (mL, STP)
PVA LA	100	1.0	40	0.37
	150	0.2	40	0.32
DLA	100	1.0	40	0.34
	150	0.2	40	0.46
RD1333	120	0.2	40	0.40

Thermal stability

No change observed in purity or brisance after storage @ 50 °C for 25 months[8], no decrease in brisance after 15 months storage @ 80 °C[8], no change in purity or brisance observed after storage under an EtOH/water mixture @ RT[8], no dec. on storage for prolonged periods of time at moderately high temperatures[33], usually stored under water for long term storage but is usually dextrinated to prevent increase in crystal size[33], threshold of thermal stability = ~200 °C, charges in primers retain explosive properties after 6 h at this temperature[41], has a tendency to slowly decompose under ambient conditions[54]

Decomposition of SLA[16]:

Trial conditions				Dec. rate loss of azide % per month
T (°C)	Humidity (% R.H.)	Other variables	Duration (months)	
60	Ambient	-	12	0.03
60	Ambient	RD1333	12	0.03
60	95	–	6	0.25
80	95	–	1	4–5
80	77	–	2	1
80	Ambient	-	1	0.05
90	50	–	0.5	5
90	Ambient	-	1	0.5–1.0
80	95	In proximity to Na_2CO_3	1	55
80	95	In CO_2	1	40

<table>
<tr><td></td><td>Stable in storage even at moderately elevated T[29], unchanged purity and brisance after 25 months storage @ 50 °C[30], unchanged purity and brisance after storage under EtOH/H_2O mixture @ RT[30], no decrease in brisance after storage @ 80 °C for 15 months[30]

14.57% weight loss after 24 h @ 181 °C (RD1333)[45]

0.15 mg (0.44%) mass loss of LA during 228 days accelerated aging @ 84 °C in vacuum (equivalent to 7.6 years at 66 °C)[58], thermal analysis of LA after 183 days of accelerated aging (equivalent to 6.1 years) shows no significant changes in DTA/TGA[58], DLA stored for ~25 years in 50:50 H_2O/EtOH showed no significant change in sensitivity to heat[61]</td></tr>
<tr><td>Sublimation rate</td><td>DLA, values marked with * are based on the data taken during the first 20 h of testing[58]:

<table>
<tr><th>T (°C)</th><th>Wt. loss rate (mg/h)</th><th>Sublimation rate (g/cm^2/s)</th></tr>
<tr><td>120</td><td>1.43×10^{-3}</td><td>6.02×10^{-10}</td></tr>
<tr><td>140</td><td>2.0×10^{-3}</td><td>7.42×10^{-10}</td></tr>
<tr><td>160</td><td>5.0×10^{-2}*</td><td>2.10×10^{-8}*</td></tr>
<tr><td>180</td><td>7.5×10^{-2}*</td><td>2.78×10^{-8}*</td></tr>
</table></td></tr>
<tr><td>Enthalpy of soln. [kcal/mol]</td><td>15.94 (α-LA)[67]</td></tr>
<tr><td>Solubility [g/mL]</td><td>0.05 g/100 g H_2O @ 20 °C[2], practically insoluble in cold H_2O, NH_3 and most common organic solvents[15], dec. in boiling H_2O[15], soluble in sodium acetate solns., ammonium acetate solns., acetic acid, ethanolamine[15], 0.02% w/w in H_2O[16], sparingly soluble in cold H_2O[20], hot H_2O dissolves enough LA to allow crystallization on cooling[20], dissolves in aqueous ammonium acetate solutions[20], some solubility in aq. ammonium acetate soln.[29], very slightly soluble in H_2O[29, 30], very soluble in acetic acid[30], almost insoluble in Et_2O, acetone, EtOH, NH_3 and common organic solvents[30], soluble in monoethanolamine or 50/50 monoethanolamine/NH_3 mixture[30]

100 g H_2O @ 18 °C dissolve 0.03 g LA[20], 100 g H_2O @ 80 °C dissolve 0.09 g LA[20]

<table>
<tr><th rowspan="2">T (°C)</th><th colspan="2">Solubility of LA (g) in 100 mL solvent[15]</th></tr>
<tr><th>H_2O[15]</th><th>Conc. aq. sodium acetate soln.[15]</th></tr>
<tr><td>18</td><td>0.023</td><td>1.54</td></tr>
<tr><td>70</td><td>0.090</td><td>–</td></tr>
<tr><td>80</td><td>–</td><td>2.02</td></tr>
</table></td></tr>
</table>

<table>
<tr><td></td><td>K_1 (solubility product) = 1.8 × 10^{-9} @ 20 °C (solubility measurements)[16], K_1 (solubility product) = 2.58 × 10^{-9} @ 25 °C (EMF measurements)[16]

0.026 g/100 g H_2O @ 20 °C (colloidal LA, 99.0 +% purity)[60], 1.0 g/100 g H_2O (special-purpose LA, RD1333, 98.5% purity)[60], 1.0 g/100 g H_2O (DLA, 91.5% purity)[60], soluble in ammonium acetate and acetic acid[67]</td></tr>
<tr><td>Hygroscopicity</td><td>0.8% @ 30 °C with 90% RH (DLA)[2], 0.03% @ 30 °C with 90% RH[2], DLA is more hygroscopic than LA[23], moderately hygroscopic[29], only slightly hygroscopic[33], very slightly hygroscopic (RD1333 LA)[44]

@ RT, 90% RH, 56 h: 1.18 (DLA, type I, US)[8], 0.07 (SLA)[8], 0.02 (CLA, type II, US)[8], 0.03 (PVA-LA, US)[8]

Hygroscopicity of spheroidal and conventional DLA[59]:

<table>
<tr><td rowspan="2">Property</td><td colspan="6">Batch no. or product</td></tr>
<tr><td>1</td><td>2</td><td>3</td><td>4</td><td>5</td><td>DUP</td></tr>
<tr><td>Purity (%)</td><td>92.90</td><td>93.16</td><td>94.43</td><td>91.98</td><td>93.44</td><td>91.50</td></tr>
<tr><td>Moisture (%)</td><td>0.46</td><td>0.61</td><td>0.57</td><td>0.66</td><td>0.74</td><td></td></tr>
<tr><td>Bulk ρ (g/mL)</td><td>2.15</td><td>2.17</td><td>2.21</td><td>2.12</td><td>2.27</td><td>1.86</td></tr>
<tr><td>Hygroscopicity</td><td>1.00</td><td>0.98</td><td>0.63</td><td>1.19</td><td>0.99</td><td>0.87</td></tr>
</table>

DUP = abbreviation for DuPont DLA</td></tr>
<tr><td>Photosensitivity</td><td>Light sensitive[15], turns yellow to dark gray in sunlight[15], darkens on exposure to light[53]

Effect of photosensitivity on ignition temperature[53]:

<table>
<tr><td>T (°C)</td><td>Normal induction period (s)</td><td>Induction period of exposed azide (s)</td></tr>
<tr><td>373</td><td>1.6</td><td>0.9</td></tr>
<tr><td>361</td><td>1.8</td><td>1.3</td></tr>
<tr><td>347</td><td>4.4</td><td>2.9</td></tr>
</table>

Irradiation of DLA had no effect on the thermal induction period but increased the % of ignitions @ 301 °C from 0% to 30%[53]

Weak photoconductor[67], critical light energy for ignition = ~29 J (light flash of ~50 µs)[67]</td></tr>
</table>

<table>
<tr>
<td>Radiation sensitivity</td>
<td>
Low dosage X-ray dose causes deterioration of LA crystals[8], higher X-ray dose produces severe crystal damage[8], 98% destruction of SLA after X-ray dose of 3.5×10^8 Roentgen[8]

Data obtained for explosives after exposure to gamma radiation[36]:

<table>
<tr><td>Weight of sample (g)</td><td>2</td></tr>
<tr><td colspan="2">Vol. of gas produced (mL/g) in following times (days)</td></tr>
<tr><td>10</td><td>1.10</td></tr>
<tr><td>20</td><td>1.95</td></tr>
<tr><td>30</td><td>2.90</td></tr>
<tr><td>40</td><td>3.95</td></tr>
<tr><td>50</td><td>5.30</td></tr>
<tr><td>90</td><td>–</td></tr>
<tr><td>Total irradiation time (days)</td><td>52</td></tr>
<tr><td colspan="2">Purity of sample by chemical analysis (%)</td></tr>
<tr><td>Original material</td><td>93.08</td></tr>
<tr><td>Irradiated material</td><td>89.04</td></tr>
<tr><td colspan="2">Melting points, corrected (°C)</td></tr>
<tr><td>Original material</td><td>–</td></tr>
<tr><td>Irradiated material</td><td>–</td></tr>
<tr><td colspan="2">IS (P.A. apparatus) (in)</td></tr>
<tr><td>Original material</td><td>3</td></tr>
<tr><td>Irradiated material</td><td>3</td></tr>
<tr><td colspan="2">IS (B.M. apparatus, 2 kg mass) (cm)*</td></tr>
<tr><td>Original material</td><td>65</td></tr>
<tr><td>Irradiated material</td><td>75</td></tr>
<tr><td colspan="2">Sand test, 200 g bomb, g of sand crushed when sample was ignited by black powder fuse only</td></tr>
<tr><td>Original material</td><td>20.5</td></tr>
<tr><td>Irradiated material</td><td>18.7</td></tr>
<tr><td colspan="2">Sand test, 200 g bomb, g of sand crushed when sample was initiated by 0.30 g LA</td></tr>
<tr><td>Original material</td><td>–</td></tr>
<tr><td>Irradiated material</td><td>–</td></tr>
</table>
</td>
</tr>
</table>

Slow neutron irradiation of lead azide[63]:

Density (g/mL)	Flux (n/cm^2/s)	Total atoms (per mL)	Metal nuclei reacting (per s)	Nitrogen nuclei reacting (per s)	Nuclear reaction
1.875	2×10^7	2.71×10^{22}	17	8×10^5	lead reactions unimportant, nitrogen reaction

Fission-fragment irradiation of LA coated with 1 μm ^{235}U[63]:

T (°C)	flux (m/cm^2 s)	^{235}U atoms per mL coating	fissions per mL sample per h	Result
150	3×10^7	7×10^{17}	4×10^7	No explosion
225	4×10^7	7×10^{17}	5×10^7	No explosion
280	3×10^7	7×10^{17}	4×10^7	No explosion
290	2×10^7	7×10^{17}	4×10^7	No explosion

Pulsed reactor irradiation of LA/boron mixtures[63]:

Ratio LA/Boron	Density (g/mL)	Neutron environment	Result
100:1	2.0	1.5×10^{15} nvt, E>10 keV 0.5×10^{15} nvt, thermal	Detonation
	2.5		Detonation
	3.0		Detonation
	3.5		Detonation

Ratio LA/Boron	Density (g/mL)	Neutron environment	Result
50:1	2.0	3.5×10^{14} nvt, E>10 keV 1.2×10^{14} nvt, thermal	No detonation
	2.5		No detonation
	3.0		No detonation
	3.5		No detonation
	2.0	3.0×10^{14} nvt, E>10 keV 1.0×10^{14} nvt, thermal	No detonation
	2.5		No detonation
	2.0	9.0×10^{14} nvt, E>10 keV 3.0×10^{14} nvt, thermal	Detonation
	2.5		Detonation
10:1	3.0	3.0×10^{14} nvt, E>10 keV 1.0×10^{14} nvt, thermal	No detonation
	3.5		No detonation
	3.0	9.0×10^{14} nvt, E>10 keV 3.0×10^{14} nvt, thermal	Detonation
	3.5		Detonation

LA irradiated at ambient T using 0.41 MeV $^{198}_{79}$Au γ-rays; volumes of gas produced measured during and after irradiation, amount of gas evolved as function of gamma dose, total gamma dose that DLA received was 5.77×10^7 R[63]:

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

Effect of gamma irradiation on various LA; [a]dose rate – ^{60}Co gamma, 3.2×10^5 R/h[63]:

Lead azide	Gamma radiation dose (R)[a]		
	Control	1.0×10^8	1.16×10^9
Dextrinated			
Color: powder	White	Dark gray	Yellow
Color: pellet	White	Dark brown	Light brown
Weight loss (%): powder		–7.5	–14.5
Weight loss (%): pellet		–0.9	–9.2
IS, p.a., 10% reactions (in)	7	6 >	36 (powder)
			>36 (pellet)
Vacuum stability (ml/g/40 h @ 100 °c)	0.47	1.35	0.57
RD1333			
Color: powder	White	Dark gray	Brown
Color: pellet	White	Dark brown	Light brown
Weight loss (%): powder		–6.4	
Weight loss (%): pellet			
IS, p.a., 10% reactions (in)	6	6	11 (powder) 16 (pellet)
Vacuum stability (ml/g/40 h @ 100 °c)	0.38	7.18	2.06
PVA			
Color: powder	White	Dark gray	Brown
Color: pellet	White	Dark brown	Brown
Weight loss (%): powder		–7.8	–14.0
Weight loss (%): pellet		–15	
IS, p.a., 10% reactions (in)	8	4	11 (powder) 21 (pellet)
Vacuum stability (ml/g/40 h @ 100 °c)	0.28	5.58	1.04

Effect of 60 MeV electron irradiation on explosives, [a]put on hot plate with *T* above explosion *T*, [b]samples tested at 100 cm with NOL apparatus[63]:

Weight (mg)	Dose (R)	Dose rate (R/s)	Weight loss	Color change	Test	Results
25.0	1.14×10^9	1.6×10^6	None	Dark brown	Heat[a]	Explosion
4.0	3.65×10^{10}	2.9×10^6	None		Heat	No explosion
11.0	2.94×10^{10}	2.7×10^6	None		Heat	No explosion
12.8	1.14×10^{10}	1.1×10^6			Impact[b]	No explosion
19.3	1.37×10^{10}	2.3×10^6	9%		Impact	No explosion

Critical doses and *T* to initiate LA by pulsed high-energy electrons, [a]estimated 50% initiation dose[63]:

Explosive	Critical dose (J/g)		Ignition *T* (°C)	
	Calcd.	Exptl.[a]	Calcd.	Exptl.
LA	158.2	46	57	327–360

Initiation of LA by pulsed electrons[63]:

Type of LA	Sample			Responses produced		Average dose to LA (J/g)	
	Density (g/mL)	Thickness (in)	Gas pressure	Number initiated	Number surviving	High surviving sample	Lowest initiate sample
Dextrinated	2.78	0.030	1 atm	1	8	124.6	150.7
	2.80	0.060	1	6	9	92.1	83.7
	2.82	0.090	1	4	11	100.5	92.1
	2.80	0.060	2 µm	9	5	46.0	41.9
	2.82	0.090	2	11	2	6.7	10.0
RD1333	2.95	0.060	1 atm	3	9	92.1	96.3
	2.95	0.060	2 µm	3	0	0	23.0

Minimum ignition energies of LA by light flashes, [a]small quantity placed in a heated aluminum block and exploded within 30 s[63]:

Compound	Color	Thermal ignition T (°C)[a]	Electrical energy of flash, half-life 0.8 ms (J)	Light intensity (J/cm^2)
LA	Yellow-white	350	240	2.0

Light-flash ignition energies for LA and its mixtures[63]:

Explosive	Critical flash ignition energy (J)
LA	28.8
LA + 0.1% graphite	32.0
LA + 0.35% graphite	34.0
LA + 1.65% graphite	52.0

Behavior of LA with a pulsed neodymium-glass (10, 600 Å) laser of 100 mW, emitting 30-nsec flashes, sensitivity to heat and nuclear reaction[63]:

Compound	Average energy densities	
	No reaction (mJ/cm^2)	100% initiation (mJ/cm^2)
LA	1.5	10

Compatibility	Dry LA does not react with or corrode steel, Fe, Ni, Al, Pb, Zn, Cu, Sn, Cd, steel, stainless steel, brass, bronze unaffected by 6 years contact @ RT or 50 °C[2], dry LA does not affect Monel, chrome-nickel and Inconel in 2 ½ years @ RT or 50 °C[2], dry LA does not affect coatings of acid-proof black paint, oil or shellac[2], LA in the presence of moisture corrodes Zn and with Cu with which it forms copper azide[2], wet LA does not affect Monel, chrome-nickel or Inconel (0.5% moisture) after 29 months @ RT or 50 °C[2], wet LA (0.5% moisture) very slightly corrodes J-1 magnesium–aluminum alloy[2], LA corrodes Cu[8], dry LA does not affect metals[33], moist LA rapidly corrodes Zn and Cu[33], incompatible with HMX (DSC)[45]

Contact atmosphere and dec. compounds identified by X-ray diffraction[16]:

Contact atmosphere	Compounds identified by X-ray diffraction			
	Residual LA	Basic lead azides	Lead carbonates	Others
Air (30–40% rel. humidity)	Mainly	Zero	As SLA†	Zero
Air and hydrochloric acid	Trace	Zero	–	Mainly $PbCl_2$
Air and acetic acid	Mainly	Zero	As SLA†	Considerable, unknown
Air and nitric acid	Mainly	Zero	AsSLA†	Some, unknown
Air and dinitroresorcinol	Mainly	Zero	As SLA†	Zero
Air and ammonia	Mainly	Zero	As SLA†	Some, unknown
Air and hydroxylamine	Mainly	Zero	AsSLA†	Zero

† *SLA = service lead azide*

Contact atmosphere and dec. compounds identified by X-ray diffraction[16]:

Contact atmosphere	Duration of trial	Compounds identified by X-ray diffraction			
		Residual LA	Basic lead azides	Lead carbonates	Others
Air and water	4 weeks	Trace	Mainly	–	–
Air + H_2O + aq. HNO_3	4 weeks	Trace	Mainly	–	–
Air + H_2O + aq. Hcl	4 weeks	Some	Much	–	–
Air + H_2O	3 days	Some	Much	As SLA†	–
Air + H_2O + dinitroresorcinol	3 days	Some	Zero	As SLA†	D compound
Air + H_2O	1 day	Much	Much	As SLA†	Zero
Air + H_2O + acetic acid	1 day	Much	Much	As SLA†	Zero
Air + H_2O + acetic acid + CO_2	1 day	Much	Trace	Much	Zero
Air + H_2O	1 week	Some	Mainly	As SLA†	Zero
Air + H_2O + ammonia	1 week	Zero	Trace	Mainly	Zero
Air + H_2O + *N*-phenyl-β-naphthylamine	1 week	Zero	Mainly	As SLA†	Trace

† *SLA = service lead azide*

DLA stored underwater must be bacteria-free water that attacks dextrine[29], may react with copper, zinc or alloys containing such metals to form azides which are more sensitive than LA[29], LA corrodes copper in presence of moisture to form cupric azide, therefore direct contact with copper or its alloys must be avoided[30]

Compatibility of DLA with black powder, 100 °C vacuum stability test, cc/40 h[2]:

Sample wt. (g)	Material	cc
1.0	LA	0.50
1.0	Black powder	0.38
2.0	50/50 LA/black powder	1.26

compatibility of LA; 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[36]:

Magnesium		N
Aluminum	A	N
Zinc	C	N
Iron		N
Steel	C	N
Tin	A	N
Cadmium	C	
Copper	D	N
Nickel	C	
Lead		N
Cadmium plated steel		
Copper plated steel		N
Nickel plated steel		N
Zinc plated steel		N
Tin plated steel		N
Magnesium aluminum	VS	
Monel metal	C	N

Brass	D	N
Bronze		N
18–8 stainless steel	A	N
Titanium		N
Silver		N

Typical compatibility of LA with various materials[63]:

Material	Compatibility	Material	Compatibility
LA RD1333		LA dextrinated	
Tungsten	Good	Zinc	Good
Molybdenum	Good	Sodium bicarbonate	Good
Tungsten disulfide	Fair	Orange shellac	
Boron nitrate	Good		
Talc	Good		
Molybdenum disulfide	Good		
Aluminum silicate hydrate	Good		

Specific heat [cal/g/°C]	0.110 @ −50 °C[2], 0.110 @ 0 °C[2], 0.110 @ 25 °C[2], 0.110 @ 50 °C[2]
Thermal conductivity [cal/s/cm/°C]	1.55×10^{-4}[2], 4×10^{-4} cgs. units (pressed pellet, mean $T = 45$ °C, pellet density = 3.62 g/cc)[67]
Hardness [kg mm^{-2}]	119.7 ± 8.0 (α-LA, single crystals, ~200 μm diameter, @ 20 °C, Vicker's hardness)[31]
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)
0.28	2.9×10^6 Pa	0.26 ± 0.04	0.26 ± 0.04		0.28

Dielectric constants

Dielectric constants and losses versus crystal orientation (α-LA)[32]:

Orientation	k'	k''	ω
<100>	17 ± 1.7	$< 2 \times 10^{-2}$	10^2–10^6
<010>	120 ± 12.0	$< 2 \times 10^{-1}$	10^2–10^6
<001>	40 ± 4.0	$< 4 \times 10^{-2}$	10^2–10^6

Reflectance tests

Reflectance tests @ 10,600 Å (continuous wave yttrium garnet aluminum laser, pressed explosive)[37]:

Material	Particle size (mesh)	Loading pressure (10^3 psi)	Reflectance (%)
Dextrinated LA	Unknown	2	86.3
	Unknown	10	79.3
Polyvinyl alcohol LA	Unknown	2	85.5
	Unknown	10	86.5

Laser sensitivity

Mean energy and energy density to initiate LA (dextrinated) with the neodymium laser[37]:

Reflectance, %	unit	Full beam		Partial beam	
		Short pulse (450 µs)	Long pulse (1.5 ms)	Short pulse (450 µs)	Long pulse (1.5 ms)
36.3	Loading pressure: 2,000 psi				
	Energy, J	1.96	3.6	2.0	3.52
	Energy density (J/in^2)	31.4	32.2	32.1	31.5
79.3	Loading pressure: 2,000 psi				
	Energy, J	1.60	2.75	1.6	2.75
	Energy density (J/in^2)	25.7	24.6	25.7	24.6

Mean energy and energy density to initiate polyvinyl alcohol LA with the neodymium laser, particle size = unknown[37]:

Reflectance, %	unit	Full beam		Partial beam	
		Short pulse (450 µs)	Long pulse (1.5 ms)	Short pulse (450 µs)	Long pulse (1.5 ms)
85.5	Loading pressure: 2,000 psi				
	Energy (J)	1.43	2.65	1.5	2.80
	Energy density (J/in^2)	22.9	23.7	24.1	25.0
86.5	Loading pressure: 10,000 psi				
	Energy, J	1.30	2.15	1.22	2.12
	Energy density, J/in^2	20.9	19.2	19.4	19.6

LA can be successfully initiated using a UV excimer laser[38]:

Pressing force (KN)	Detonator type	Nominal wavelength (nm)	Energy density (KJ/m^2)	Function time (micro-s)	Source	Pulse duration (µs)
1	Confined	249	0.2	0.5	Excimer laser	15
10	Confined	249	0.2	1.5	Excimer laser	15

Detonation conditions using laser-produced heat and shock; Neodynium/glass laser[38]:

Density of pressing force (g/cc)	Detonator type	Nominal wavelength	Spot diameter (µm)	Power or energy (J)	Function time (µs)	Pulse duration (µs)
2.0	Confined	1,060	600	0.004	262	250
2.0	Confined	1,060	600	0.080	170	250

Sensitiveness	4.76 N cm^2 (work)[42]

M50 detonator transition charge test

Data from[44]

Transition material	Charge weight (mg)	RDX weight (mg)	Test holder	Witness material	Indent depth (in)
LA	110	34	Brass	Aluminum	0.0548
LA	110	34	Brass	Aluminum	0.0483
LA	110	34	Brass	Aluminum	0.0485
LA	110	34	Brass	Lead	0.1975
LA	110	34	Brass	Lead	0.2144
LA	110	34	Plastic	Lead	0.1362
LA	110	34	Plastic	Lead	0.1429

Strong confinement test

LA, RD 1333, data from[44]:

Loading pressure (kpsi)	Average charge density (g/cm^3)	Average dent (mils)
5	2.62	27.7
10	2.99	33.7
20	3.18	39.0
40	3.55	46.3

@ 10 kpsi loading pressure[44]: $\rho = 3.119\ g\ cm^{-3}$, dent = 37.3 mils[44]

Hot wire initiation test

30 unit Bruceton run with P-12 units loaded with 20 mg of test material; constant current Bruceton – current applied for 10 s. in steps of 10 mA, current constant to ± 2%; capacitor discharge Bruceton – used 0.1 or 1.0 mfd capacitor and 0.3 log unit voltage steps, LA RD1333, data from[45]

Bridge	Constant current			Cap discharge	
Tophet C	Mean (amps)	AF 99.9% (amps)	NF 0.1% (amps)	Mean (V, mF)	Stored energy (mJ)
0.001	0.299 ± 0.009	0.326	0.272	79.99 ± 3.44, 1.0	3.20
0.0005	0.132 ± 0.008	0.157	0.108	143.55 ± 35.84, 0.1	1.03

<table>
<tr><td></td><td>RD1333 LA, data from[46]

<table>
<tr><td rowspan="2">Bridge (mm)</td><td colspan="3">Constant current</td><td colspan="2">Capacitor discharge</td></tr>
<tr><td>Mean (mA)</td><td>All fire (99.9%)</td><td>No fire (0.1%)</td><td>Mean (V, mF)</td><td>Stored energy (mJ)</td></tr>
<tr><td>0.0254</td><td>299 ± 9</td><td>326 mA</td><td>272 mA</td><td>79.99 ± 1.04, 1.0</td><td>3.20</td></tr>
<tr><td>0.0127</td><td>132 ± 8</td><td>157 mA</td><td>108 mA</td><td>143.55 ± 1.25, 0.1</td><td>1.03</td></tr>
</table></td></tr>
<tr><td>Priming ability</td><td>200 mg RDX, pressed @ 10 kpsi in Al cup, 0.01–0.10 g RD-1333 sample, plastic spacer to hold fuse, seal can at top of can, 1,020 steel plate dent block (1” outer diameter, 0.5” thick), PMMA holder (1.25” long, 1” outer diameter); loose charge of 0.010 g RD1333 insufficient to cause detonation of RDX charge, larger loads of 0.025 g or 0.40 g gave go no-go results[45]: level 50_0 (gms) = 0.0288, σ_0 = 0.0093[45]

Minimum primary charge = 10 mg, actual charge = 20–30 mg (5 mm thick lead plate, LA filled in no. 8 blasting cap, pressed by 32 MPa static pressure, fired by standard pyrotechnical igniter)[55]</td></tr>
<tr><td>Ignition sensitivity by electric bridge current</td><td>Bridge current and ignition time (I = ignition current (ampere); s, ignition time (1/1,000 s); I^2s = (ignition current)^2 × (ignition time))[48]:

<table>
<tr><td>I</td><td>2.0</td><td>1.6</td><td>1.3</td><td>1.0</td></tr>
<tr><td>s</td><td>2.1</td><td>4.0</td><td>6.5</td><td>13.1</td></tr>
<tr><td>I^2s</td><td>8.4</td><td>10.2</td><td>11.0</td><td>13.1</td></tr>
</table></td></tr>
<tr><td>Flame test</td><td>Flame sensitivity H_{50} <8 cm (H_{50} reflects the reliability of ignition)[55]</td></tr>
</table>

Initiation energies for electrostatic initiation of LA; [a] kilohms, [b]megaohms[62]:

LA type	Apparatus and electrodes	Gap length (mm)	Discharge	Capacitance (pF)	Series Resistance (ohms)	Rel. Humidity (%)	Energy (J)
RD1333	Approaching needle plane	0	contact	300	0	dry	$<6 \times 10^{-8}$
						75	3.8×10^{-5}
						40	3.0×10^{-6}
				1,000			$<3 \times 10^{-5}$
		0.48	Gaseous	3,000		12	$3–6 \times 10^{3}$
		0.25		50			$<5 \times 10^{-5}$
		0.19		2,000		Dry	3.6×10^{-3}
		0.19		1,200	100 K[a]		3.5×10^{-4}
	Needle rubber	?		1,000		40	$<5 \times 10^{-4}$
	fixed gap needle plane	0.25	Gaseous	300	0	Dry	$1–2 \times 10^{3}$
		1.1		10,000		55	2×10^{-2}
		0.13		330		40	1.3×10^{-3}
		0.13			1.2 M[b]		2×10^{-4}
	Parallel plate	0.19			0		3.3×10^{-4}
		0.19			1.2 M		1.1×10^{-4}
	Vibrator needle	0.03	Contact	50	0	9	4×10^{-10}
Service	Approaching needle plane	0	Contact	100	0	40	2.0×10^{-6}
					20 K		1.6×10^{-6}
		0.04	Gaseous	1,500	100 K		2.2×10^{-4}

	Needle rubber			500			1.0×10^{-3}
				1,500			2.2×10^{-4}
Dextrinated	Approaching needle plane	7	Gaseous	300	0	dry	$7–9.6 \times 10^{-3}$
		7		7			7.0×10^{-3}
		0	Contact	7	7		1.0×10^{-5}
		0.75	Gaseous	7	0		1.0×10^{-2}
		9		1,000			$3–4.5 \times 10^{-3}$
		?		20,000			1.0×10^{-2}
		?		1,000			$1–4.5 \times 10^{-3}$
	Plumb-bob plane	0	Contact	300			2.0×10^{-5}
	Needle rubber	7	Gaseous	10,000	100 K		8.0×10^{-2}
		7		10,000			$0.5–1.0 \times 10^{-1}$
	Plumb-bob rubber	7		6,000			2.0×10^{-3}
	Fixed gap needle plane	1.3		10,000	100		$2–3 \times 10^{-2}$
		1.1		10,000	0		2.0×10^{-2}
	Parallel plane	0.19		550	5.6 M		5.0×10^{-4}
PVA	Approaching needle plane	0	Contact	7	7		2.0×10^{-7}
		7	Gaseous	7	7		6.3×10^{-3}
	Needle (neg.) Rubber	7		400	100 K	40	2.2×10^{-4}
	Needle (pos.) Rubber	7		200			1.0×10^{-4}
	Fixed gap needle plane	1.1		10,000	0	55	2.0×10^{-2}
		1.3		1,000	100	40	$3–4 \times 10^{-3}$

	α-$Pb(N_3)_2$[8, 9, 32]	β-$Pb(N_3)_2$[9]	α-$Pb(N_3)_2$[10]	β-$Pb(N_3)_2$[10]	α-$Pb(N_3)_2$[67]	β-$Pb(N_3)_2$[67]
Chemical formula	N_6Pb	N_6Pb	N_6Pb	N_6Pb	N_6Pb	N_6Pb
Molecular weight [g mol^{-1}]	291.26	291.26	291.26	291.26	291.26	291.26
Crystal system	Orthorhombic	Monoclinic	Orthorhombic	Monoclinic	Orthorhombic	Monoclinic
Space group	*P c m n*		*P n m a* (no. 62)	*C* 2 (no. 5)		
a [Å]	11.31	18.49	6.63	18.49	6.63	5.09
b [Å]	16.25	8.84	16.25	8.85	11.31	8.84
c [Å]	6.63	5.12	11.31	5.12	16.25	17.51
α [°]	90		90	90	90	90
β [°]	90		90	107.6	90	90.10
γ [°]	90		90	90	90	90
V [$Å^3$]	1,218.51		1,218.51	798.601		
Z	12		12	8	12	8
ρ_{calc} [g cm^{-3}]	4.68	4.87	4.76267	4.84461		
T [K]	RT		RT			

lead azide forms four allotropes: *α*-, *β*-, *γ*-, *δ*-[15], however only the α- allotrope has found technical applications[15], monoclinic (*β*-form) is much more sensitive than orthorhombic (*α*-form)[30]

Crystals of orthorhombic *α*-form can be obtained from ammonium acetate or acetic acid soln.[67], monoclinic *β*- form crystals can be obtained by allowing lead and azide ions to diffuse slowly together[67]

Comparison of the properties of the four LA allotropes[15]:

α	β	γ	δ
– Orthorhombic – $\rho = 4.68–4.716$ (crystal) – Formation of α allotrope promoted by addition of dextrin at precipitation point – Most stable allotrope	– Monoclinic – $\rho = 4.87–4.93$ (crystal, dry) – Long needles (crystals) – Formation of *β*-allotrope promoted by presence of organic dyes (e.g., Eosin, erythrosine, neutral red) at precipitation point – Stable – Irreversible transformation to α-LA @ ~160 °c	– Monoclinic – ΔH_f is 1.25 kJ/mol higher than that of α-form – obtained by maintaining pH in 3.5–7.0 range – Usually precipitates simultaneously with δ-LA – Forms in the presence of polyvinylalcohol	– Triclinic – Obtained by maintaining pH in 3.5–5.5 range – Usually precipitates simultaneously with γ-LA

Known polymorphs[16]: *α* (common rhombic form), $\rho = 4.7$ g cm^{-3}
β (monoclinic), $\rho = 4.9$ g cm^{-3}
γ (monoclinic), $\rho = 4.7$ g cm^{-3}
δ (triclinic), $\rho = 4.6$ g cm^{-3}

α-$Pb(N_3)_2$, orthorhombic, space group probably $Pc2_1n$[16]:

Z	*a* (Å)	*b* (Å)	*c* (Å)	ref.
12	11.34	16.25	6.64	*Miles* (1931)
	11.312	16.246	6.628	*Pfefferkorn* (1948)
	11.42	16.30	6.65	*Duke* (1951)
12	11.31	16.25	6.63	*Azaroff* (1956)
	11.41	16.31	6.67	*Hattori and McCrone* (1956)
	11.330	16.271	6.636	*Lemnevik and Söderquist* (1963)

β-$Pb(N_3)_2$, monoclinic, *I*-centered cell, space group either *I*2/*m* or *I*2[16]:
I-centered cell[16]:

Z	*a* (Å)	*b* (Å)	*c* (Å)	*β* (°)	Ref.
8	17.60	8.83	5.10	90.8	*Miles* (1931)
	17.508	8.844	5.090	90.2	*Pfefferkorn* (1948)
	17.569	8.837	5.113	90.29	*Lemnevik and Söderquist* (1963)

C-centered cell[16]:

Z	*a* (Å)	*b* (Å)	*c* (Å)	*β* (°)	Ref.
8	18.37	8.89	5.11	106.3	*Duke* (1951)
	18.49	8.84	5.12	107.6	*Azaroff* (1956)
	18.31	8.88	5.23	107.5	*Hattori and McCrone* (1956)
	18.323	8.837	5.113	106.5	*Lemnevik and Söderquist* (1963)

γ-$Pb(N_3)_2$, monoclinic, formation of γ-$Pb(N_3)_2$ favored by low pH and/or presence of polyvinyl alcohol at appropriate rates of crystallization[16]:

Z	*a* (Å)	*b* (Å)	*c* (Å)	*β* (°)	Space group	Ref.
8	12.17	10.51	6.55	98.5	$P2_1/a$	*Duke* (1957)
	12.060	10.507	6.505	95.75	$P2_1/m$ or $P2_1$	*Lemnevik and Söderquist* (1964)

δ-$Pb(N_3)_2$, triclinic, formation of δ-$Pb(N_3)_2$ favored by low pH and/or the presence of polyvinyl alcohol at appropriate rates of crystallization[16]:

Z	*a* (Å)	*b* (Å)	*c* (Å)	*α* (°)	*β* (°)	*γ* (°)	Ref.
8	15.163	10.532	6.531	90.53	98.12	112.67	*Lemnevik and Söderquist* (1964)

"We think, however, that there is an anomaly in the results for γ-lead azide … A possible explanation may be that these two forms are related as polytypes, and that some degree of variability exists in the crystals[16]"

Cubic phase[16]: "it has not been possible to obtain this phase in a reproducible manner or in a pure state. Its identity is not known, it may or may not be lead azide; it is not lead nitrate (primitive cubic lattice, $a = 7.856$)" (*Duke*, 1951, 1953 cited in ref.[16]).

Basic lead azide[16]: "Analysis agrees with the composition PbN_3OH, monoclinic, probably $P2_1/c$, $a = 15.25$ Å, $b = 5.75$ Å, $c = 14.47$ Å, $\beta = 114.7°$ (crystal data), $\rho = 6.19$ (observed), $\rho = 6.14$ (calcd.) X-ray powder data[16]

Spontaneous explosion during crystal growth of LA (LA dissolved in 50 mL of 5% aqueous ammonium acetate soln. @ 70 °C then allowed to cool to RT within 2 h without disturbance)[16]:

LA (%)	Time to explosion (min)	LA (%)	Time to explosion (min)
1.0	40 ± 2	0.7	210
1.0	50	0.7	220
0.9	75	0.6	225
0.9	65	0.6	255
0.8	80	0.5 (10 expts.)	7 × exploded overnight (large α- crystals in intact containers)
0.8	85	0.4 (4 expts.)	No explosions after 4 days standing, no crystals separated

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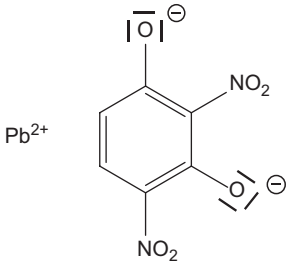
Lead 2,4-dinitroresorcinol

Name [German, acronym]: Lead 2,4-dinitroresorcinate, [Blei 2,4-dinitroresorcinat, PbDNR, 2,4-LDR, LDNR]

Main (potential) use: Primary explosive, ingredient of priming mixtures[1], component of compositions for electric detonators[1, 4, 5], patented for use as delay or priming composition[9]

Structural formula:



	LDNR
Formula	$PbC_6H_2N_2O_6$
Molecular mass [g mol^{-1}]	405.30
Appearance at RT	Two forms known: (i) yellow solid, (ii) orange-red solid[1, 4], red or yellow crystals[3, 4], red or yellow solid[5], precipitated as a mixture of colloidal (smaller quantity) and crystalline forms[9], extremely free-flowing brown almost spherical granules[9]
IS [J]	30 cm (1 kg hammer)[1], 30 cm (1 kg mass, 20 mg sample, B.M.)[4], 20 in (2 kg mass, P.A.)[4], 30 cm (1 kg mass, B.M.)[5], 63 cm (0.5 kg mass, 34 ± 1 mg sample, ERL machine)[7], 22 cm (1.0 kg mass, 34 ± 1 mg sample, ERL machine)[7], 9 cm (2.5 kg mass, 34 ± 1 mg sample, ERL machine)[7], 61 cm (median height, FoI = 11 (standard), 2 kg mass, Rotter apparatus)[8]
FS [N]	FS tested on porcelain and Emery paper (Julius-Peters, BAM)[2]:

Friction sensitivity (g)					
Porcelain	Emery paper Grades				
	P80	P100	P120	P180	P360
115	150	100	125	330	550

Emery paper FS[8]:

Ignitions/trial at strike velocity (ft/s)					Type of ignition
5	6	7	8	9	
1/10	4/10	7/10	7/10	8/10	Complete

Sliding block FS, with steel on steel surfaces, substantially the same results were obtained with a dead load of 40 lb instead of 6 lb on the tilting table[8]:

Explosive surface	Ignitions/trial at velocity strike (ft/s)									
	5	6	7	8	9	10	11	12	13	14
Steel on steel	0/10	3/10	5/10	8/10	10/10	10/10				
Emery				0/10	1/10	5/10	7/10	5/10	9/10	9/10

ESD [J]

Threshold ignition energies[6]:

Metal/metal electrodes (no added circuit resistance)		Rubber/metal electrodes (105 ohm series resistance)	
Contact sparks (500 pf)	Gaseous sparks (1,000 pf)	Minimum energy	Minimum capacity (pf)
–	–	1,250	25

N [%]	6.91
$\Omega(CO_2)$ [%]	–32
$T_{m.p.}$ [°C]	265 (explodes)[6]
$T_{dec.}$ [°C]	
ρ [g cm^{-3}]	3.2 (crystal)[4, 6], 1.02 (bulk density of extremely free-flowing brown granules with average particle size of 0.10 mm)[9], 0.95 (bulk density, average particle size of 0.10 mm)[9]
Heat of formation	–396.01 kJ/mol (standard enthalpy of form.)[10]

	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]			270 cal/g[4, 6]

T_{ex} [K]			
$p_{C\text{-}J}$ [kbar]			
VoD [m s^{-1}]			
V_0 [L kg^{-1}]			
Trauzl test [cm^3, % TNT]	41.7% TNT[1]		
Sand test [g]	20 g (200 g bomb)[5]		
Initiating efficiency	0.4 g does not initiate tetryl[1], 0.4 g does not initiate tetryl pressed @ 3,000 psi[4], Sensitivity of LDR in wire bridge initiators, W wire 0.030 in long fired @ 14–20 V[6]: 138 Erg for 0.0001 in diameter[6], 930 Erg for 0.00029 in diameter[6]		
5 s explosion *T* [°C]	265[4, 5]		
100 °C heat test [% mass loss]	0.20% mass loss in first 48 h[4], 0.02% mass loss in second 48 h[4], no explosion in 100 h[4]		
Vacuum stability test [cm^3/h]	Explodes in 73 min @ 120 °C[4]		
Solubility [g/mL]	Insoluble in H_2O, acetone, benzene and other common organic solvents[1]		
Hygroscopicity	Stored wet[3], 0.73% @ 30 °C and 90% RH[4], only slightly hygroscopic[5]		

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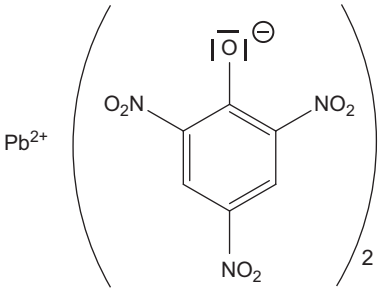
Lead picrate

Name [German, acronym]: Lead(II) 2,4,6-trinitrophenolate, [Bleipikrat, Blei(II)-2,4,6-trinitrophenolat]

Main (potential) use: Component of ignition mixtures in the WW-II[1], component of mixtures for electric fuse heads[1], component of cap compositions for the manufacture of electric fuses in the WW-II[6]

Structural formula:



Normally lead picrate contains 1–5 molecules of H_2O[1]; anhydrous lead picrate forms the monohydrate if exposed to air[1]*, heating the •H_2O or •4H_2O salt @ 150 °C produces the anhydrous salt*[1, 6]

	Lead picrate
Formula	$C_{12}H_4N_6O_{14}Pb$ (anhydrous)
Molecular mass [g mol^{-1}]	663.41
Appearance at RT	Anhydrous = yellow solid[1], silky yellow needles (tetrahydrate)[6]
IS [J]	4 cm (0.5 kg mass, anhydrous)[1], higher sensitivity than MF[1], anhydrous more sensitive than hydrates[1], 97 cm (detonates, 750 g, air-dry condition of sample)[3]
N [%]	12.67
Ω(CO_2) [%]	
$T_{m.p.}$ [°C]	
$T_{dec.}$ [°C]	
ρ [g cm^{-3}]	
Heat of formation	

	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{ex}U^{o}$ [kJ kg^{-1}]			
T_{ex} [K]			
$p_{C\text{-}J}$ [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)[3]		
5 s explosion T [°C] 1 s explosion T [°C] ignition T [°C]	 281[1] 263[4], 283 (instant)[4]		
Burn rate [mm/s]	Burning rate @ 100 atm. gauge = 26 cm/s[2], and @ 300 atm. gauge = ~31 cm/s[2], below a certain pressure the burn rate rapidly decreases and burning is then extinguished @ 20 atm.[2]		
Solubility [g/mL]	Anhydrous lead picrate insoluble in H_2O, Et_2O, $CHCl_3$, benzene, toluene[1], sparingly soluble in acetone, EtOH[1]		
Ignition sensitivity by electric bridge current	Bridge current and ignition time (I = ignition current (ampere), s = ignition time (1/1,000 s), I^2s = (ignition current)^2 × (ignition time))[4]:		

I	2.0	1.6	1.3	1.0	0.8	0.6
s	4.3	5.6	6.1	9.1	11.0	31.6
I^2s	17.2	14.4	10.5	9.1	7.0	11.4

	$[Pb_2(pic)_4(dmso)_4]$[5]
Chemical formula	$C_{32}H_{32}N_{12}O_{32}Pb_2S_4$
Molecular weight [g mol^{-1}]	1,639.4
Crystal system	Triclinic
Space group	*P*-1 (no. 2)
a [Å]	10.1003(6)
b [Å]	11.2872(9)
c [Å]	11.6147(9)
α [°]	77.868(2)

β [°]	89.884(2)
γ [°]	84.785(2)
V [Å^3]	1,289
Z	1 (dimer)
ρ_{calc} [g cm^{-3}]	2.112
T [K]	ca. 153
	DMSO solvate of lead(II) picrate, clusters of yellow needle-like crystals

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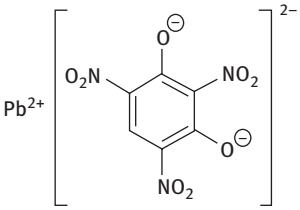
Lead styphnate

Name [German, acronym]: Lead styphnate, lead(II) 2,4,6-trinitrobenzene-1, 3-bis(olate), lead trinitroresorcinate, lead salt of 2,4,6-Trinitrobenzene-1,3-diol [Bleistyphnat, Bleitrizinat, Blei trinitroresorcinat, tricinate, LTNR, LS]

Main (potential) use: Primary explosive, igniting charge, in mixtures for blasting caps[11], component of pyrotechnic mixtures for primers[11], fusehead composition component[11], ingredient of priming layer that causes LA to explode from a flash[13], mainly found in primers[17], primary explosive used in friction-type primers[19], in cap and detonator compositions[30]

Structural formula: *



** Normal lead styphnate forms as a hydrate*[11]

	LS
Formula	$C_6HN_3O_8Pb \cdot H_2O$
Molecular mass [g mol^{-1}]	468.3
Appearance at RT	Orange reddish-brown solid[1], yellow-orange or reddish-brown rhombic, needle-like crystals[2], crystallizes as gold-orange or red-brown monohydrate crystals[11], reddish-brown, short, rhombic crystals[13], crystalline material varies in color from straw, deep yellow, orange-yellow or red-brown[19], reddish-brown solid[21], yellow – light brown small crystals[30]

IS [J]

17 cm (2 kg mass, B.M.)[1, 21], 3 in (8 oz mass, P.A.)[1], 2.5–5 Nm[3, 28], 3 in (2 kg mass, P.A.)[21], <20 kg-cm[27], 69 cm (median height, 2 kg mass, 30 mg sample, Rotter apparatus[41], anhydrous more sensitive than normal LS[11], storing LS for 60 days @ 75 °C increased the IS from 23 cm–5 cm (1 kg hammer)[11], 2.2[11], 2.5[11], 2.4[11], 3.4 (B.M.)[11], ~3.5[11], 5[11], H_{50} = 2.16 (8.8 cm, 2.5 kg mass)[11], minimum hot spot *T* for initiation by impact = 500–550 °C (in the presence of grit)[14], 0.025 (basic LS)[17], 22.1 ± 4.1 cm (ball drop, steel ball, ball weight = 8.36 g, 50% height)[22], 8 in (22 mg sample, P.A.)[24], FoI = 25[30], $H_{10\%}$ = 12 in (ball drop test, 8.35 g, ½ in diameter steel ball, 35 mg sample)[32], $H_{50\%}$ = 15 in (ball drop test, 8.35 g, ½ in diameter steel ball, 35 mg sample)[32], 0.025[36], 36 cm (100% fire, 400 g hammer, 20 mg sample)[37], 11.5 cm (100% no-fire, 400 g hammer, 20 mg sample)[37], 20.3 cm (P.A.)[38], 69 cm (median height, 2 kg mass, FoI = 12 cf. Pb 2,4-DNR = 11, Rotter apparatus)[38]

Silver sand test (crystalline LTNR, 16.27 g falling mass)[31]:

Test *T* (°C)	50	40	30	–1	–11	–21	–30	–41
Critical height (cm)	6.9	7.7	7.6	10.1	11.3	11.9	12.1	12.7

Grain size and IS of lead trinitroresorcinol, silver sand test (@ RT, 16.27 g falling mass)[31]:

Grain size (sieve mesh)	Height of fall (cm)	No. of explosions (per 40 shots)	Critical height of fall (cm)
300 or more	13 11	22 16	12.0
300–200	11 9	23 19	9.5
200–150	15 12	23 15	13.8
150–80	15 12	22 16	14.0
80 or less	20 17	21 18	18.9

Impact initiation delay, delay range is for approx. 20 initiations[38]:

Impact energy (J)	Average delay (µs)	Delay range (µs)
6.34	133	60–200
4.80	193	80–990
3.40	191	70–420

Effect of liquid nitrogen on the IS (2 kg mass, modified P.A. machine, 50% point, *T* cycling = soaking sample in LN_2 for 15 min. then allowing to stand at ambient *T* for 1 h for five cycles)[38]:

	Height (cm) (standard deviation)
Mean height for 50% probability of reaction	
Control (dry)	33.43 (13.39)
LN_2 test	32.16 (4.52)
Height for 10% probability of reaction	
Control (dry)	15.24
LN_2 test	17.78
Effect of *t* cycling at 50% height	
In LN_2, % fire	60
Dry, % fire	30

FS [N]

Detonates with steel shoe (friction pendulum test)[1, 24], detonates with fiber shoe (friction pendulum test)[1], minimum hot spot *T* for initiation by friction = 430–500 °C (in the presence of grit)[14], <1 (basic LS)[17], <1 kg (BAM)[27], 0.1[28], 1.45 (50% initiation probability)[11], less sensitive than mercury fulminate[30], <1[36], 70% (explosion % of 25 samples under 588.40 kPa and 80° swing angle)[37], explodes in Picatinny Arsenal friction test[38]

FS tested on porcelain and Emery paper (Julius-Peters, BAM)[16]:

Friction sensitivity (g)					
Porcelain	Emery paper grades				
	P80	P100	P120	P180	P360
275	450	240	200	375	> 2,075

F_{50} = 1.3 (dry sample) (FSKM-PEx OZM friction tester, roughened ceramic plate and porcelain peg)[18], F_{50} = 7.69 (5% water) (FSKM-PEx OZM friction tester, roughened ceramic plate and porcelain peg)[18], F_{50} = 20.05 (10% water) (FSKM-PEx OZM friction tester, roughened ceramic plate and porcelain peg)[18], F_{50} = 30.14 (20% water) (FSKM-PEx OZM friction tester, roughened ceramic plate and porcelain peg)[18], F_{50} = 28.56 (excess water) (FSKM-PEx OZM friction tester, roughened ceramic plate and porcelain peg)[18]

$F_{50\%}$ = 285 ± 200 g (Julius-Peters, BAM, porcelain plate and peg, Bruceton method)[22], $F_{10\%}$ = 100 g (Julius-Peters, BAM, porcelain plate and peg, Bruceton method)[22]

Emery paper FS[39]:

Ignitions/trial at strike velocity (ft/s)				Type of ignition
8	9	10	11	
0/10	3/10	7/10	9/10	complete

Sliding block F, with steel on steel surfaces, substantially the same results were obtained with a dead load of 40 lb instead of 6 lb on the tilting table[39]:

Explosive and surface	ignitions/trial at velocity strike (ft/s)									
	5	6	7	8	9	10	11	12	13	14
LS steel on steel	0/10	0/10	0/10	0/10	0/10	0/10	0/10	0/10	0/10	0/10
LS Emery					0/10	1/10	1/10	5/10	5/10	9/10

Effects of liquids on sliding block FS, sliding block friction tester with 6 lb load, no. of ignitions at 14 ft/s, Perminal = sodium salt of isopropyl naphthalene sulfonic acid[39]:

Desensitizer	Ignitions/trial
Without desensitizer	10/10
Sprayed 20 s w/water or w/20% glycerin soln.	6/10
Same plus 0.1% perminal	6/10
Same, plus 0.1% turkey red oil	5/10
One drop EtOH	0/10

Yamada FS apparatus[39]:

Explosive and additive	Load for 50% initiations (kg)		
	Emery	Ebonite	Copper
LS	20.0	35.0	
LS, ground glass 100 mesh	15.5	32.0	100

<table>
<tr><td>ESD [J]</td><td>
<5 kV[27], 0.0009[1, 37], 0.001[2], 0.04–0.14 mJ[11], 0.2 mJ (basic LS)[17], 0.0009 (unconfined)[24, 38], 0.0009 (confined)[24, 38], 0.2 mJ[28, 36]

Highest electrostatic discharge energy @ 5,000 V for zero ignition probability[7]:

<table>
<tr><td colspan="2">Highest energy (J) for zero ignition probability</td><td colspan="2">Type of ignition</td></tr>
<tr><td>Unconfined</td><td>Confined</td><td>Unconfined</td><td>Confined</td></tr>
<tr><td>0.0009</td><td>0.0009</td><td>deton.</td><td>deton.</td></tr>
</table>

Ignition values[23]:

<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>LS</td><td>0.001</td><td>3.7</td><td>0.007</td><td>30</td><td>54</td><td>Ignited</td></tr>
</table>

Threshold ignition energies, the gaseous and contact spark regions of sensitiveness are continuous with LS; the energy value quoted is the energy (erg) stored on the capacitor – the energy dissipated in the gap is about one-tenth of this[24]:

<table>
<tr><td rowspan="2">Material</td><td colspan="2">Metal/metal electrodes (no added circuit resistance)</td><td colspan="2">Rubber/metal electrodes (105 ohm series resistance)</td></tr>
<tr><td>Contact sparks (500 pF)</td><td>Gaseous sparks (1,000 pF)</td><td>Minimum energy</td><td>Minimum capacity (pF)</td></tr>
<tr><td>LS</td><td>60</td><td>–</td><td>20</td><td>5</td></tr>
</table>
</td></tr>
<tr><td>N [%]</td><td>8.97</td></tr>
<tr><td>Ω(CO_2) [%]</td><td>–22.2</td></tr>
<tr><td>$T_{m.p.}$ [°C]</td><td>260–310 (explodes)[1, 20, 21, 24], detonates before melting[19]</td></tr>
<tr><td>$T_{dec.}$ [°C]</td><td>260–310 (explodes, DSC @ 5 °C/min)[1], 295.61 (DSC, LTNR prepared with batch experiment)[12], 293.38 (DSC, LTNR prepared with segmented experiment)[12], 304.99 (DSC, LTNR prepared with segmented experiment with 5% glycerin)[12], 282 (DSC, basic LS)[17], 282 (exo peak max, DSC)[28], 282 (DSC)[36]</td></tr>
</table>

Normal LS, exptl. features of the DSC traces[33]:

	Endotherm	Exotherm
Heating rate = 2.5 K/min Mass of sample = 0.525 mg, 0.510 mg		
T_{onset} (K)	405	533
T_{max} (K)	414	552
Heat of reaction (J/g)	65	1,890
Heating rate = 5 K/min Mass of sample = 0.486 mg, 0.508 mg		
T_{onset} (K)	416	542
T_{max} (K)	425	560
Heat of reaction (J/g)	59	1,930
Heating rate = 10 K/min Mass of sample = 0.469 mg, 0.465 mg		
T_{onset} (K)	423	554
T_{max} (K)	434	571
Heat of reaction (J/g)	75	2,010
Heating rate = 20 K/min Mass of sample = 0.463 mg, 0.447 mg		
T_{onset} (K)	436	564
T_{max} (K)	447	580
Heat of reaction (J/g)	69	2,010

ρ [g cm^{-3}]

3.02 (crystal)[1, 2, 20, 24], 3.06–3.1 (crystal, normal LS)[11], 2.9 (anhydrous LS)[2, 11, 20], 3.00 (basic LS)[17], 3.1 (crystal)[22, 28], 2.47 @ 12,000 psi[24], 3.09[30], 3.00[36]

Loading ρ at different pressures[5, 24]:

Pressure (kpsi)	Loading ρ (g cm^{-3})
3	2.12[5, 24]
5	2.23[5, 24]
10	2.43[5, 24]
15	2.57[5, 24]
20	2.63[5, 24]
crystal	3.1[5, 24]

Heat of formation	−1,786.9 kJ/kg (enthalpy of form.)[3], −1,747.2 kJ/kg (energy of form.)[3], −738.27 ± 6.95 kJ/mol ($\Delta_f H^o$, calorimetry)[6], 92.3 cal/g[2], 92 kcal/kg[9], −835 kJ/mol (normal LS)[11], −92 cal/g[1]		
Heat of combustion	1,251 kcal/kg[1, 2, 9, 24]		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{ex}U^o$ [kJ kg^{-1}]	2,322	457 kcal/kg[9] 725 kJ/mol[11]	457 cal/g[1, 24] 460 cal/g [H_2O (g)][2]
T_{ex} [K]	2,955	2,700 °C[9]	
$p_{C\text{-}J}$ [kbar]	244		0.126 Mbar[24]
VoD [m s^{-1}]	6,098 (@ 3.02 g cm^{-3}, $\Delta_f H = -624$ kJ mol^{-1})	5,200 (@ 2.9 g cm^{-3}, average value from lit.)[8] 2,100 (@ 0.93 g cm^{-3})[11] 4,900 (@ 2.6 g cm^{-3})[11] 5,200 (@ 2.9 g cm^{-3})[11] 6,200 (@ 3.1 g cm^{-3})[11]	5,200 (@ 2.9 g cm^{-3})[1, 20, 21] 5,200 (@ 2.9 g cm^{-3}, when initiated with blasting caps)[2] 4,802 (based on sand experiments)[8] 4,900 (@ 2.6 g cm^{-3}, loaded into detonator capsules, 7.7 mm internal diameter, *Kast*)[13] 4,900 (@ 2.6 g cm^{-3})[30]
V_0 [L kg^{-1}]	344	270 dm^3/kg[11]	368[1, 24] 440[2]

Trauzl test [cm^3, % TNT]	40% TNT[1, 21], more powerful than LA[2], 42% TNT[2], 130 cm^3 (10 g sample)[11], 122 cm^3 (10 g sample)[11], 40% TNT (10 g sample)[11]
Sand test [g]	27–53% TNT[2], 10.9 g sand crushed (1,700 g bomb using 0.4 g LS)[8], 24 g (200 g bomb)[1, 21], 10.5 g (initiation by black powder fuse)[2], 24 g (initiated by small charge of MF)[2]

<table>
<tr><td>Initiating efficiency</td><td>Trace of MF is minimum detonating charge[1], trace of LA is minimum detonating charge[1], 0.001 g minimum detonating charge of LA[24], 2 g of LS does not initiate tetryl[11], minimum charges of LS required to initiate 0.4 g PETN (PETN tamped down or pressed loosely into Cu capsules, 6.2 mm inside diameter, LS pressed down loosely on top, values given for 1 failure in 10 tests achieved): 0.55 g[13], minimum charges of LS required to initiate 0.4 g PETN (PETN compressed @ 2,000 kg/cm^2), Cu capsules, 6.2 mm inside diameter, LS pressed down loosely on top: no detonation with 1 g LS[13], initiating ability = <0.5 g (minimum charge in a No. 8 detonator for tetryl)[28], LS is a relatively poor initiator of detonation: detonation of 60% dynamite and gelatin dynamite is possible[2], the only military explosive LS detonates is unpressed PETN, minimum detonating charge for unpressed PETN = 0.55 g[2], 0.001 g (minimum detonating charge of LA required to shock-initiate LS)[38]</td></tr>
<tr><td>5 s explosion T [°C]
Explosion T [°C]</td><td>282[1, 2, 21, 37], 270–280[9], 282 (cook-off)[24], 282 (open cup)[38]

276 (10 s)[1, 24], 272 (15 s)[1], 267 (20 s)[1], instantaneous explosion @ 270 (Kast)[11], 276 (glass tube, 20 °C/min)[13], 277 (glass tube, 20 °C/min)[13], 276 (iron tube, 20 °C/min)[13], 275 (iron tube, 20 °C/min)[13], 265 (iron tube, 65 s)[13], 270 (iron tube, 0 s)[13]

Explosion T @ various times of exposure (3 mg samples, detonation)[10]: 0.56 s @ 328, 4.47 s @ 301, 41.3 s @ 280, no action @ 275[10]

Time to explosion of LS as function of time (approx. values)[11]:

<table>
<tr><th>T (°C)</th><th>Time to explosion (min)</th></tr>
<tr><td>235</td><td>36</td></tr>
<tr><td>238</td><td>23</td></tr>
<tr><td>239</td><td>26</td></tr>
<tr><td>241</td><td>22</td></tr>
<tr><td>242</td><td>21</td></tr>
<tr><td>242</td><td>17</td></tr>
<tr><td>243</td><td>22</td></tr>
<tr><td>246</td><td>19</td></tr>
<tr><td>248</td><td>14</td></tr>
<tr><td>250</td><td>13</td></tr>
<tr><td>253</td><td>9</td></tr>
<tr><td>255</td><td>8</td></tr>
</table>
</td></tr>
</table>

5 s ignition *T* [°C] Ignition *T* [°C]	267–268 (explodes, 0.05 g sample in test tube in Wood's metal bath, @ 20 °C/min)[13] 282 (US value)[9, 24], 265–280 (Russian value) (explodes)[9], 280 (Danilov)[11] 293 (dropping on preheated Wood's alloy)[5], 255 (@ 5 °C/min)[11], 275–277 (@ 20 °C/min)[11], 250[14], ~250 (@ 5 °C/min)[30], 295 (crystalline)[31], 299 (powder)[31], 300 (anhydrous)[31], 298 (grain size = ≥300 sieve mesh)[31], 295 (grain size = 300–200 sieve mesh)[31], 297 (grain size = 200–150 sieve mesh)[31], 298 (grain size = 150–80 sieve mesh)[31], 298 (grain size = ≤80 sieve mesh)[31], 530 K[33], 324 (5 s, extrapolated)[35], 440 (10^{-3} s, extrapolated)[35], 522 (10^{-5} s, extrapolated)[35]
Detonating *T* [°C]	267[19]
Autoignition *T* [K]	522[22], 280 °C (DSC @ 10 °C, hermetic sealed ups and lids)[27]
Thermal ignition *T* [°C]	250[24]
100 °C heat test [% mass loss]	0.38% mass loss in first 48 h[1], 0.73% mass loss in second 48 h[1], no explosion in 100 h[1], 1.5% mass loss (may be due to loss of crystal H_2O)[2], 0.4 cc/40 h @ 100 °C[2], 40 cc/40 h @ 120 °C[2]
Vacuum stability test [cm^3/h]	0.4 cm^3 gas evolved in 40 h @ 100 °C[1, 2], 0.4 cm^3 gas evolved in 40 h @ 120 °C[2], 0.3 cm^3 gas evolved in 40 h @ 120 °C[1, 24, 38]
Thermal stability	Loss in weight @ 105 °C: 0.02% after 3 h[1], 0.23% after 6 h[1], 0.23% after 9 h[1] Effect of storage for 2 months @ 80 °C on (i) explosion temperature test value = none[1], (ii) sand test value = none[1], (iii) sensitivity to initiation = none[1] Storage @ 80 °C caused no change in 100 °C VTS value[2], normal LS (LS•H_2O) shows no change after 2 months @ 65–70 °C[11], heating (LS•H_2O) >100 °C results in loss of crystal water[11], dehydration of LS•H_2O after 16 h @ 115 °C[11], dehydration of LS•H_2O after 7 h @ 135 °C[11], dehydration of LS•H_2O after <4 h @ 145 °C[11], 267–268 (explodes, 0.05 g sample in test tube in Wood's metal bath, @ 20 °C/min)[13], detonates if steamed[19], storage @ 80 °C doesn't affect its stability[20]

<table>
<tr><td>Burn rate [mm/s]</td><td>Linear and mass rates of burning @ 1 atm[29]: $u = 26–27$ cm/s[29], $m = 100$ g cm^{-2} s^{-1}[29], $u = \approx 25–26$ cm/s @ 15 mm Hg pressure in bomb[29], $u = \approx 33–35$ cm/s @ 50 atm. and remains unchanged @ 50–400 atm.[29]</td></tr>
<tr><td>Solubility [g/mL]</td><td>0.1 g soluble in 100 g glycol diacetate @ 20–25 °C[1], 0.04 g/100 g H_2O @ 15 °C (slightly soluble)[2, 11], 0.09 g/100 g H_2O @ 17 °C (slightly soluble)[11], slightly soluble in MeOH, pyridine, amyl acetate[11], practically insoluble in Et_2O, acetone, $CHCl_3$, CCl_4[11, 20], soluble in formamide, ethanol diamine (30 g/100 g ethanol diamine @ 17 °C)[11], slightly soluble in H_2O[19], less soluble in acetone[19], some solubility in 10% aq. ammonium acetate soln.[19, 20], practically insoluble in water, EtOH, carbon disulfide, benzene, toluene, hydrochloric acid and glacial acetic acid[20], insoluble in Et_2O, $CHCl_3$, CCl_4, CS_2, benzene, toluene, conc. hydrochloric acid and glacial acetic acid[2], soluble in aqueous ammonium acetate[2]</td></tr>
<tr><td>Hygroscopicity</td><td>0.05% @ 25 °C with 100% RH[1], 0.02% @ 30 °C with 90% RH[1], normal LS is hygroscopic (LS•H_2O)[11], heating (LS•H_2O) >100 °C results in loss of crystal water[11], dehydration of LS•H_2O after 16 h @ 115 °C[11], dehydration of LS•H_2O after 7 h @ 135 °C[11], dehydration of LS•H_2O after <4 h @ 145 °C[11], slightly hygroscopic[19], only slightly hygroscopic[21]</td></tr>
<tr><td>Radiation sensitivity</td><td>Dec. on γ-irradiation, cobalt-60 @ 25 °C[11]

Data obtained for explosives after exposure to gamma radiation[24]:

<table>
<tr><td>Weight of sample (g)</td><td>5</td></tr>
<tr><td colspan="2">Vol. of gas produced (mL/g) in following times (days)</td></tr>
<tr><td>10</td><td>0.05</td></tr>
<tr><td>20</td><td>0.07</td></tr>
<tr><td>30</td><td>0.09</td></tr>
<tr><td>40</td><td>–</td></tr>
<tr><td>50</td><td>0.10</td></tr>
<tr><td>90</td><td>0.12</td></tr>
<tr><td>Total irradiation time (days)</td><td>90</td></tr>
<tr><td colspan="2">Purity of sample by chemical analysis (%)</td></tr>
<tr><td>Original material</td><td>–</td></tr>
<tr><td>Irradiated material</td><td>–</td></tr>
<tr><td colspan="2">Melting points, corrected (°C)</td></tr>
<tr><td>Original material</td><td>–</td></tr>
<tr><td>Irradiated material</td><td>–</td></tr>
</table>
</td></tr>
</table>

IS (P.A. apparatus) (in)	
Original material	6
Irradiated material	6
IS (B.M. apparatus, 2 kg mass) (cm)	
Original material	20
Irradiated material	22
Sand test, 200 g bomb, g of sand crushed when sample was ignited by black powder fuse only	
Original material	14.1
Irradiated material	14.3
Sand test, 200 g bomb, g of sand crushed when sample was initiated by 0.30 g LA	
Original material	–
Irradiated material	–

Effects of reactor irradiation, [a]average reactor exposure rates: fast neutrons ϕ >0.18 MeV 1.4×10^{13} n/cm^2 s, thermal neutron ϕ >0.17 eV 8.6×10^{13} n/cm^2 s, gamma 4.0×10^8 R/h (3.38×10^{10} ergs/g(C)(h gamma), [b]sample detonated, [c]200 °C[40]:

Irradiation time (min)	Total neutron dose		Total gamma (R)	Weight loss (%)	10% loss on TGA (°C)	150° avg. gas evolution (mL/g/hr)	DTA peak exotherm @ 20 °C/min (°C)	5 s explosion *T* (°C)
	Fast (n/cm^2)	Thermal (n/cm^2)						
0					285	1.02[c]	287[b]	299
~2	1.7×10^{15}	1.1×10^{15}	1.4×10^7			Sample detonated		
~1 ms	7.3×10^{13}	2.2×10^{14}	3.6×10^6	0.26		2.53 [c]	280[b]	268
~1 ms	3.5×10^{14}	1.6×10^{15}	1.5×10^7			Sample detonated		

Radiation sensitivity

LS irradiated at ambient *T* using 0.41 MeV $^{198}_{79}$Au γ-rays; volumes of gas produced measured during and after irradiation, amount of gas evolved as function of gamma dose[40]:

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

Effect of 60 MeV electron irradiation on explosives, [a]put on hot plate with *T* above explosion *T*[40]:

Weight (mg)	Dose (R)	Dose rate (R/s)	Color change	Test	Results
25.0	1.14×10^9	1.1×10^6	Dark rust-brown	Heat[a]	Explosion
25.0	1.14×10^9	1.6×10^6		Heat	Explosion
3.3	3.65×10^{10}	2.9×10^6		Heat	No Explosion
7.9	2.96×10^{10}	2.7×10^6		Heat	Explosion
10.3	22.7×10^{10}	2.9×10^6		Heat	Explosion

Critical doses and *T* to initiate LS by pulsed high-energy electrons, [a]estimated 50% initiation dose[40]:

Explosive	Critical dose (J/g)	
	Calcd.	Exptl.[a]
LS	92.1	42

Compatibility

Compatible with RDX, tetryl, TNT when dry[11], slightly hygroscopic but not adversely affected by moisture[19], can be stored under H_2O or under a mixture of H_2O/EtOH[19], does not react with copper, aluminum, stainless steel, LA or black powder[19], detonates if steamed[19], no reaction and no corrosion with Al[24], no reaction with Cu[24], no reaction with 18–8 stainless steel[24]

Blast wave characteristics

Blast wave overpressure P_{max} = 3.0 kPa (mean value)[15], blast wave positive phase impulse I^+ = 0.25 Pa s (mean value)[15] (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)[15], TNT equivalence = 0.42[15]

Specific heat [cal/cm/°C]

0.141 @ −50 °C[1], 0.158 @ 0 °C[1], 0.164 @ 25 °C[1], 0.167 @ 50 °C[1]

Firing times of hot bridge wire initiators

Firing times of hot bridge wire initiators, 50 mg loads of explosives, voltage of 450 V, times are in μs[24]:

Milling times (h)	Capacitance (μF)		
	0.5	0.05	0.0047
24	11.8–12.5	10.0–20.6	13.1–374.4
64	10.0–13.7	10.6–13.1	10.0–381.2

Reflectance tests

Reflectance tests @ 10,600 Å (continuous wave yttrium garnet aluminum laser, pressed explosive)[25]:

Particle size (mesh)	Loading pressure (10^3 psi)	Reflectance (%)
Through 100	2	65.3
Through 100	10	76.8

Laser sensitivity

Mean energy and energy density to initiate LS with the neodymium laser[25]:

Particle size (mesh)	Reflectance (%)	Unit	Full beam		Partial beam	
			Short pulse (450 μs)	Long pulse (1.5 ms)	Short pulse (450 μs)	Long pulse (1.5 ms)
Through 100	65.3	Loading pressure: 2,000 psi				
		Energy (J)	0.56	0.98	0.58	0.98
		Energy density (J/in^2)	9.0	8.8	9.3	8.8
Through 100	76.8	Loading pressure: 10,000 psi				
		Energy (J)	0.45	0.85	0.53	0.87
		Energy density (J/in^2)	7.2	7.6	8.5	7.8

LS can be successfully initiated using a UV excimer laser[26]:

Pressing force, KN	Detonator type	Nominal Wavelength (nm)	Energy density (KJ/m^2)	Function time (μs)	Source	Pulse duration (μs)
1	Confined	249	0.6	220	Excimer laser	15
10	Confined	249	0.6	750	Excimer laser	15

Detonation conditions using laser-produced heat and shock[26]:

Density or pressing force	Detonator type	Nominal wavelength (nm)	Spot diameter (µm)	Power or energy (J)	Energy density (J/M^2)	Function time (µs)	Laser type	Pulse duration (µs)
10.3 MPa	Confined	1,060	600	0.070	–	273	Neodymium /glass	250
14 MPa	Confined	820	200	1	30	250	Diode	100,000
~1 g/cc	Confined	820	200	1	30	250	Diode	27,500

Pulsed nedodymium-glass (10,600 Å) laser of 100 MW emitting 30 ns flashes[40]:

Average energy densities	
No reaction (mJ/cm^2)	100% initiation (mJ/cm^2)
100	1,200

Ignition sensitivity by electric bridge current

Bridge current and ignition time (I = ignition current (ampere), s = ignition time (1/1,000 s), I^2s = (ignition current)^2 × (ignition time))[31]:

Crystalline lead trinitroresorcinol						
I	2.0	1.6	1.3	1.0	0.8	0.75
s	1.4	2.1	3.4	6.4	20.6	
I^2s	5.6	5.4	5.7	6.4	13.2	
Powder lead trinitroresorcinol						
I	2.0	1.6	1.3	1.0	0.8	0.75
s	1.8	2.6	3.9	6.9	26.3	
I^2s	7.2	6.7	6.6	6.9	16.8	
Anhydrous lead trinitroresorcinol						
I	2.0	1.6	1.3	1.0	0.8	0.75
s	1.7	2.7	4.0	8.3	22.0	
I^2s	6.8	6.9	6.8	8.3	14.1	

Heat of dec. [J/g]

1890 (DSC @ 2.5 K/min)[33], 1930 (DSC @ 5 K/min)[33], 2010 (DSC @ 10 K/min)[33], 2010 (DSC @ 20 K/min)[33], 1960 ± 70 (average value, DSC)[33]

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[34]:

Sample	T_0–T_{po} (ms)	T– T_{pk} (ms)	T_{p0}- T_{pk} (ms)	Ignition time (ms)*	Peak pressure (psi)	Charge weight (g)	Impetus (in lb/g)
NLA	0.785	1.034	0.250	0.734	1,361	0.238	3,488

	Lead styphnate monohydrate*[4]
Chemical formula	$C_6H_3N_3O_9Pb$
Molecular weight [g mol^{-1}]	468.3

Crystal system	Monoclinic
Space group	
a [Å]	10.06
b [Å]	12.58
c [Å]	8.05
α [°]	90
β [°]	91.90
γ [°]	90
V [Å^3]	1,018.21
Z	4
ρ_{calc} [g cm^{-3}]	3.055
T [K]	295

** Normal LS forms a monohydrate and exists as two polymorphs: α and β*[11]

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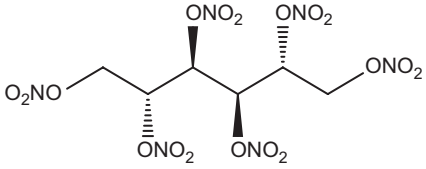
M

D-Mannitol hexanitrate

Name [German, acronym]: D-Mannitol hexanitrate, nitromannite, nitromannitol, mannitol hexanitrate, hexanitromannite, hexanitromannitol, Mannitol nitrate, Maxitate, Medemanol, Dilangil, Moloid, Mannitrin, Nitranitol, Manexin [Nitromannit, MHN, HNMnt, HNM]

Main (potential) use: Improvised explosive, secondary charge in detonators and blasting caps, its mixture with tetracene is a powerful primary explosive[15], high-explosive charge in compound detonators which contain DDNP as primary explosive[15], secondary charge in detonators and in blasting caps designed to be initiated by a fuse[4]

Structural formula:



	D-Mannitol hexanitrate
Formula	$C_6H_8N_6O_{18}$
Molecular mass [g mol^{-1}]	452.15
Appearance at room temperature [RT]	Crystallizes from EtOH as needles[14], white crystals[15], colorless crystals or white powder[17], white crystalline powder (thin needles)[18], long needles in regular clusters (from EtOH)[22]
IS [J]	1 (100–500 µm), 8–11 cm (B.M.)[8], 4 in (P.A.)[8], 11 cm (2 kg mass, 2.16 J, B.M.)[2, 3], 4 in (2 kg mass, 1.99 J, P.A.)[2, 3], similar to that of NG[14], 4 cm (explosion, 2 kg mass)[14, 15], explodes on concrete surface by hitting with hammer[15], 11 cm (2 kg mass, 20 mg sample, B.M.)[4], 4 in (2 kg mass, 11 mg sample, P.A.)[4], $H_{50\%}$ = 15 cm (4 kg mass, B.M. design 5)[24], $H_{50\%}$ = 12 cm (5 kg mass, plane sandblasted surfaces)[24], 5.5 cm (sensitivity to glancing impact, Hercules sliding rod, sandblasted surfaces, 45° slide angle, 10 lb rod, 30 mg sample)[24]

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<table>
<tr><td>FS [N]</td><td>30 (100–500 µm), detonates with steel shoe (friction pendulum test)[4], unaffected by fiber shoe (friction pendulum test)[4], $H_{50\%}$ = 1.1 cm (friction pendulum, 30 mg sample, sandblasted surface, 2 in ball, 5 kg weight, 8° angle of incidence)[24]</td></tr>
<tr><td>ESD [J]</td><td>0.15 (100–500 µm)</td></tr>
<tr><td>N [%]</td><td>18.59</td></tr>
<tr><td>$\Omega(CO_2)$ [%]</td><td>+7.08</td></tr>
<tr><td>$T_{m.p.}$ [°C]</td><td>112–113[4, 8, 14, 15, 17, 2, 18], 112[7], 109 (after several recrystallizations)[8], 109.5 (onset), 111.8 (peak max), 113.9 (end T) (DSC @ 10.0 K/min, pinhole cover)[16], 106–108[22], 109.5 (endo, onset), 111.8 (endo, peak max) (DSC 10 K/min)[25]</td></tr>
<tr><td>$T_{dec.}$ [°C]</td><td>157 (DSC @ 5 °C/min), 150[4], 150 (slow heating)[8], 150 (small quantity is heated)[15], 150 (complete dec., red fumes, no crackling, slow heating)[18], 169.4 (onset), 181.4 (peak max), 202.6 (end T) (DSC @ 10.0 K/min, pinhole cover)[16], 169.4 (exo, onset), 181.4 (exo, peak max) (DSC 10 K/min)[25]

Nonisothermal TG data[25]:

<table>
<tr><th rowspan="2">β/K min^{-1}</th><th rowspan="2">T_{ot}</th><th rowspan="2">T_i</th><th colspan="2">Mass loss/%</th><th rowspan="2">L_{max}/% min^{-1}</th><th rowspan="2">T_p/°C</th><th rowspan="2">T_{oe}/°C</th></tr>
<tr><th>Stage 1</th><th>Residue/%</th></tr>
<tr><td>7.0</td><td>155.0</td><td>127.4</td><td>96.73</td><td>0.32</td><td>–28.11</td><td>169.4</td><td>190.0</td></tr>
<tr><td>10.0</td><td>160.2</td><td>129.7</td><td>95.82</td><td>0.74</td><td>–45.41</td><td>173.3</td><td>193.7</td></tr>
<tr><td>15.0</td><td>164.2</td><td>132.3</td><td>96.83</td><td>0.79</td><td>–66.56</td><td>176.6</td><td>199.8</td></tr>
<tr><td>20.0</td><td>166.2</td><td>136.9</td><td>98.46</td><td>0.22</td><td>–76.10</td><td>180.7</td><td>214.2</td></tr>
</table>
T_{ot} = onset T of dec., T_{oe} = onset T of end 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</td></tr>
<tr><td>ρ [g cm^{-3}]</td><td>1.894 (@ 173 K), 1.784 (gas pycnometer @ 298 K), 1.73[4], 1.604[7], 1.230–1.604 (crystal)[8], sp. gr. = 1.604[14, 17, 18]</td></tr>
<tr><td>Heat of formation</td><td>–165.2 kcal/mol[8], –169.42 ± 0.68 kcal/mol[8], –1,494.4 (enthalpy of form.)[7], 337 cal/g[4], 345 cal/g[4], 366 cal/g[4], –706.7 ± 4.2 kJ/mol (–ΔH_f°, (c))[13], 342.8 kcal/kg (heat of form., Q)[18], –169.42 kcal/mol[8], 349 kcal/kg[9], –708.8 kJ/mol (enthalpy of form., exptl.)[23], –662.6 kJ/mol (enthalpy of form., calcd., emp.)[23]</td></tr>
<tr><td>Heat of combustion</td><td>–674.9 kcal/mol[8], –1,521 cal/g[8], –1,484.2 cal/g (99.46% purity)[8], 1,520 kcal/kg[9], –1,565 cal/g[8], –1,525 cal/g[4, 8], –689.5 kcal/mol (Q_c^v)[8], –683.7 kcal/mol (Q_c^p)[8], –1,515 cal/g[4, 8], 1,512 kcal/kg (@ C^v)[18], 2,844.3 kJ/mol (ΔH_c, heat of comb.)[25]</td></tr>
<tr><td></td><td></td></tr>
</table>

	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]	5,938	Heat of explosion = 1,458 kcal/kg[9] 1,512 kcal/kg[14] 1,510 kcal/kg[18] 151.6 kcal/100 g (@ 1.73 g cm^{-3}, constant volume) [H_2O (l)][20]	1,390 cal/g[4] 1,454 cal/g[4, 8] 1,468 cal/g[4] 1,520 cal/g[4] 6,380[6] 5,855 [H_2O (g)][7]
T_{ex} [K]	4,189	6,040 (@ 1.7 g cm^{-3}, calcd.)[9] 4,590 °C (@ 1.73 g cm^{-3})[20]	
$p_{C\text{-}J}$ [kbar]	296	300 (@ 1.7 g cm^{-3}, calcd.)[9]	
VoD [m s^{-1}]	8,488 (@ TMD)	8,070 (calcd., R-P method)[12] 8,260 (@ 1.73 g cm^{-3}, average value from lit.)[10] 9,010 (@ 1.593 g cm^{-3}, calcd., K-J)[16]	7,000 (@ 1.5 g cm^{-3}, iron pipe, 25 mm diameter, 5 mm wall thickness)[8] 8,260 (@ 1.73 g cm^{-3})[1, 2, 7] 8,260 (@ 1.73 g cm^{-3}, pressed, confined, 0.5 in charge diameter)[4, 5] 8,260 (@ 1.7 g cm^{-3})[10] 8,294 (calcd. from 1,700 g bomb sand test)[10] 5,600 (@ 0.9 g cm^{-3}, Fe pipe, 25/35 mm diameter)[14] 7,000 (@ 1.5 g cm^{-3}, Fe pipe, 4 mm diameter)[14] 8,260 (@ 1.75 g cm^{-3}, Fe pipe, 12.8 mm diameter)[14, 15]

V_0 [L kg^{-1}]	755	69.4 l/100 g (@ 1.73 g cm^{-3}, @ STP)[20]	755[6] 694[7] 723[8]

Trauzl test [cm^3, % TNT]	172% TNT[2, 4, 8], 150% PA, 102% NG[8], 172–196% TNT[10], 560 cm^3 (H_2O tamping)[14], 560 mL[18], 510[21]
Sand test [g]	68.5 g (200 g bomb)[2, 4], 137–143% TNT[10], 65.4 g sand crushed (1,700 g bomb, 0.4 g sample)[10], 121.5–143% TNT[8]
Ballistic mortar test	136–150% TNT[10]
Initiating efficiency	0.06 g LA minimum detonating charge[4]
SSGT [cm]	Nitromannite, TMD = 1.73 g cm^{-3}, commercial sample was received and stored wet, dried @ 120°F under vacuum overnight[19]:

Loading pressure (kpsi)	Density (g/cm^3)		% TMD	Sensitivity (DBG)			
	AVG.	S		AVG.	g	s_m	*N*
1	0.957	0.0186	55.3	1.967	0.2514	0.1269	20
2	1.113	0.0124	64.3	2.968	0.0426	0.0269	20
4	1.293	0.0081	74.7	3.103	0.0531	0.0308	20
8	1.458	0.0063	84.3	3.820	0.0401	0.0294	20

5 s explosion *T* [°C]	175[2, 4]
1 s ignition *T* [°C]	232 (US value)[4, 9], 205 (Russian value)[9]
Ignition *T* [°C]	232 (dropping on heated Wood's alloy)[11], 165[8]
Explosion *T* [°C]	160–170 (0.1 s)[4], 160–170 (heating in test tube)[14], 160–170 (deflagration on heating larger samples)[15]
100 °C heat test [% mass loss]	Frothed in 48 h[8], exploded in 100 h[8]
International heat test@ 75 °C	0.4% mass loss in 48 h[4, 8]
Thermal stability	Sample recryst. several times shows similar stability to that of NG[14], samples recryst. less often withstand 75 °C for only few hours (brown fumes evolve)[14], dec. after few hours @ 75 °C (covered glass vessel)[15], low thermal stability can be improved by addition of 0.5–3.0% ammonium salts or urea[18]

	Nonisothermal TG data, β = °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.[16]:

β (°C/min)	T_{ei} (°C)	T_p (°C)	T_{oe} (°C)	T_b (°C)
7.0	155.0	169.4	190.0	138.5
10.0	160.2	173.3	193.7	
15.0	164.2	176.6	199.8	
2ß.0	166.2	180.7	214.2	

	Stable enough to be used commercially but significantly less stable than nitroglycerol @ 75 °C[22], critical T for thermal dec. = 113.2 °C[25]
Vacuum stability test [cm^3/h]	2.62 mL gas evolved after 1 h @ 100 °C[8], 3.69 mL gas evolved after 2 h @ 100 °C[8], 6.75 mL gas evolved after 3 h @ 100 °C[8]
Solubility [g/mL]	Immiscible with H_2O[14], dissolves readily in Et_2O, hot EtOH[4, 14, 15, 17], only slightly soluble in cold EtOH[4, 15], insoluble in water[4, 15, 22], slightly soluble in Et_2O[4], readily soluble in acetone, Et_2O and hot EtOH[18], weakly soluble in cold EtOH[18], insoluble in H_2O[18], soluble in EtOH and Et_2O[22]
ΔH_{melt} [J/g]	–87.4 (heat absorption)[16]
Hygroscopicity	0.17% @ 30 °C with 90% RH[4], only slightly hygroscopic[2]
$\Delta H_{dec.}$ [J/g]	631.2 (heat release)[16], 285.4 kJ/mol (ΔH_d, heat of dec.)[25]
65.5 °C KI test	6 min[4]

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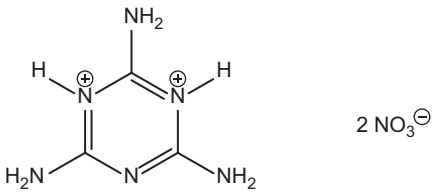
Melaminium dinitrate

Name [German, acronym]: Melaminium dinitrate, [MDN]
Main (potential) use: Patented for possible use as high temperature stable explosive[1], possibly in wellbores[1]

Structural Formula:



	MDN		
Formula	$C_3H_8N_8O_6$		
Molecular mass [g mol^{-1}]	252.15		
Appearance at RT	Crystalline solid[1], colorless crystals[2, 3]		
IS [J]	>30 (BAM)[3, 4]		
FS [N]	>350 (BAM)[3, 4]		
N [%]	44.44		
Ω(CO_2) [%]	−25.4		
$T_{m.p.}$ [°C]			
$T_{dec.}$ [°C]	330 (DSC @ 2 K/min)[4]		
ρ [g cm^{-3}]	1.852 (X-ray @ 200 K)[3, 4]		
Heat of formation	−149.8 kcal/mol ($\Delta H_f°$(s))[4]		
	Calcd.(EXPLO)	Lit. values	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]	2,977[4]		
T_{ex} [K]	2,562[4]		
$p_{C\text{-}J}$ [kbar]	236[4]		
VoD [m s^{-1}]	7,723 (@ 1.852 g cm^{-3}) [4]	8,910 (ρ not specified, calcd., R-P method)[1]	
V_0 [L kg^{-1}]	803[4]		

Thermal stability	Stable @ 137 °C for 48 h without detectable dec.[1], should be stable @ ~200 °C (wellbore temperature) for several hours[1], no dec. @ 137 °C (long-term stability measurements using RADEX)[3], stable for at least 48 h @ 140 °C (RADEX V5 oven, isothermal tempering)[4]
Solubility	soluble in MeOH, water[4]

	Melaminium dinitrate[2]	**Melaminium dinitrate[3]**
Chemical formula	$C_3H_8N_8O_6$	$C_3H_8N_8O_6$
Molecular weight [g mol^{-1}]	252.17	252.17
Crystal system	Monoclinic	Monoclinic
Space group	$P2_1/c$ (no. 14)	$P2_1/c$ (no. 14)
a [Å]	7.7710(14)	7.758(5)
b [Å]	9.8924(18)	9.804(5)
c [Å]	12.186(2)	12.094(5)
α [°]	90	90
β [°]	101.198(9)	100.53(1)
γ [°]	90	90
V [Å^3]	919.0(3)	904.4(8)
Z	4	4
ρ_{calc} [g cm^{-3}]	1.823	1.852
T [K]	100	200

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[2] L. Vella-Zarb, D. Braga, A. G. Orpen, U. Baisch, *CrystEngComm*, **2014**, *16*, 8147–8159.
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Mercury fulminate

Name [German, acronym]: Mercury fulminate [Quecksilberfulminat, Knallquecksilber, MF]

Main (potential) use: Primary explosive[17], detonators, component in percussion priming mixtures (historically)[12, 23], pyrotechnics (historically)[12], blasting caps (historically)[12, 17], fuse detonators[17, 23], detonators either as pure compound or mixed with 10–20% NO_3^-[20]

Structural formula:

$$Hg(CNO)_2$$

	Mercury fulminate
Formula	$C_2N_2O_2Hg$
Molecular mass [g mol^{-1}]	284.6
Appearance	White–gray solid[1], three forms known depending on the preparation route: (i) white, (ii) brown and (iii) gray[12], MF crystallizes from H_2O as $\bullet^1/_2$ H_2O crystals[13], obtained anhydrous from EtOH[13], heavy crystalline solid[17], white if pure but usually has slight brown-yellow or gray color[17], white (pure) or gray (manufactured)[19], octahedral truncated crystals[19], white solid (pure)[20], grayish-yellow (lower purity) solid[20], gray or brownish solid[23], light yellowish-brown (crude, 97.10% purity)[29], white (99.42% purity, crude MF treated with conc aq. NH_3 and aq. acetic acid soln.)[24], powder (crude MF soaked in water in mortar then carefully grind)[24], white diamond-shape crystal (crude MF treated with conc. aq. NH_3 and aq. acetic acid, left in dark to crystallize)[24]
IS [J]	5 cm (2 kg mass, B.M.)[1, 8, 20], 35 cm (1 kg mass, B.M.)[1], 2 in (2 kg mass, P.A.)[1, 20], 4 in (1 lb mass, P.A.)[1, 8], 0.62 (impact energy for 50% prob. of initiation)[7], $H_{60\%}$ = 7.5 cm (Wöhler app.)[4], 1–2 Nm[2], 5 mm (20 mg sample, B.M.)[9], 4 in (2.2 kg mass, P.A.)[9], 5 cm (2 kg mass)[3], 10.5 cm (500 g mass)[3], range from ~0.2–2.0[12], minimum hot spot *T* for initiation by impact = 500–550 °C (in presence of grit)[14], 2–4 cm (2 kg mass)[15, 19], 4.5 cm (2 kg mass)[13], 127 mm (500 g mass required for detonation)[13], 9–10 in (8 oz weight required for explosion)[13], F of I = 10[23]

Silver sand tester (28.5 g falling mass, white MF)[24]:

Test T (°C)	Critical height (cm)	Test T (°C)	Critical height (cm)
50	15.4	−10	23.4
40	19.4	−21	23.6
30	20.5	−29	23.9
−2	23.4	−40	24.4

Silver sand tester (28.5 g falling mass, crude MF)[24]:

Test T (°C)	Critical height (cm)	Test T (°C)	Critical height (cm)
50	15.7	−10	19.5
40	16.5	−21	19.9
30	17.5	−28	20.6
−1	18.6	−40	21.0

Silver sand tester (28.5 g falling mass, powder MF)[24]:

Test T (°C)	Critical height (cm)	Test T (°C)	Critical height (cm)
50	15.4	−11	23.2
40	16.4	−17	23.2
30	17.2	−29	23.9
0	22.4	−40	24.6

Impact initiation delay, [a] for approx. 20 initiations[27]:

Impact energy (J)	Average delay (µs)	Delay range (µs)[a]
6.34	45	22–102
4.85	38	24–104
3.40	85	24–177
1.94	112	40–300
1.29	114	50–350
0.47	196	50–630
0.20	97	40–200

Ball drop apparatus, total impulse at 50% detonations = 2.6×10^4 cgs units, time of impact @ 50% detonations = 1.9×10^{-4} s, force = $I/t = 1.37 \times 10^8$ dynes, impulsive pressure = $1.37 \times 10^8 / 0.88 \times 0.1 = 1.56 \times 10^9$ dyne cm^{-2}[29]:

Ball diameter (in)	Ball mass (g)	Height (h_1) (cm)	E	Detonations (%)	mhg (ergs × 10^{-6})	Net kinetic energy (ergs × 10^{-6})	Impulse (cgs units × 10^{-4})
3/4	28.14	60	0.738	15.0	1.65	0.75	1.67
3/4	28.14	90	0.738	31.7	2.48	1.13	2.06
3/4	28.14	120	0.739	43.3	3.30	1.50	2.38
7/8	44.66	60	0.636	45.0	2.62	1.58	2.50
7/8	44.66	80	0.627	63.3	3.50	2.12	2.89
7/8	44.66	100	0.628	85.0	4.38	2.65	3.23

FoI = 10 (Rotter apparatus, cf.. RDX FoI = 80)[30]

FS [N]

Explodes with steel shoe (friction pendulum test)[1, 9], explodes with fiber shoe (friction pendulum test)[1, 9], very sensitive[23], 5.3 (friction force for 50% prob. of initiation)[7], less sensitive than LA[3], 6.48 (white MF)[12], 7.47 (brown MF)[12]

Sliding-block FS, with steel on steel surfaces, substantially the same results were obtained with a dead load of 40 lb instead of 6 lb on the tilting table[27]:

Surface	Ignitions/trial at velocity strike (ft/s)								
	6	7	8	9	10	11	12	13	14
Steel on steel	0/10	1/10	5/10	8/10	8/10	7/10	9/10	10/10	10/10
Emery		0/10	1/10	4/10	4/10	7/10	9/10	10/10	10/10

Effect of liquids on sliding-block FS, sliding block tester with 6 lb load, no. of ignitions at 14 ft/s, Perminal is sodium salt of isopropyl naphthalene sulfonic acid[27]:

Desensitizer	Ignitions/trial
Without desensitizer	10/10
Sprayed 20 s w/water or w/20% Glycerin soln.	2/10
Same, plus 0.1% Perminal	2/10
One drop EtOH	0/10

Emery friction: 50% fires @ 4.5 ft/s[30]

<table>
<tr><td>ESD [J]</td><td>0.025[1], 0.025 (electric spark sensitivity)[8], 0.025–0.07[9], values range from 0.51–0.62 mJ to 25 mJ[12], wet MF not exploded by spark, but is exploded by dry patches of MF[13], metal/metal electrode: 150 µJ @ 5,000 pF[30]

Highest electrostatic discharge energy @ 5,000 V for zero ignition probability[10]:

<table>
<tr><th colspan="2">Highest energy (J) for zero ignition probability</th><th colspan="2">Type of ignition</th></tr>
<tr><td>Unconfined</td><td>Confined</td><td>Unconfined</td><td>Confined</td></tr>
<tr><td>0.025</td><td>0.025</td><td colspan="2">High order deflagration</td></tr>
</table>
</td></tr>
<tr><td>N [%]</td><td>9.8</td></tr>
<tr><td>$\Omega(CO_2)$ [%]</td><td>–16.86</td></tr>
<tr><td>$T_{m.p.}$ [°C]</td><td>Decomposition[1], 160 (but explodes @ this temp.)[9], detonates before melting[17]</td></tr>
<tr><td>$T_{dec.}$ [°C]</td><td>160 (but explodes @ this temp.)[9], 190 (within 20 s, Wood’s metal bath)[13]</td></tr>
<tr><td>ρ [g cm^{-3}]</td><td>4.43 (crystal)[1, 9], 4.42 (crystal)[2, 19], 1.55–1.75 (apparent)[8], 4.42–4.43 (crystal)[8, 12], 4.467 (crystal)[12], 1.35–1.55 (bulk ρ)[12], sp. gr. = 4.45[13], ~1.75 (apparent ρ, gravimetric ρ)[13], usually compressed in detonators to ~2.5[13], values up to 4.0 obtained by vigorous compression[13], 4.45[23], 1.7 (bulk ρ)[23], 3.5–4.0 (loaded ρ after being pressed into detonators)[23]

ρ if subjected to different pressures[8]:

<table>
<tr><th>Pressure (psi)</th><th>ρ (g cm^{-3})</th></tr>
<tr><td>3,000</td><td>3.0[1, 8]</td></tr>
<tr><td>5,000</td><td>3.20[1]</td></tr>
<tr><td>10,000</td><td>3.60[1, 8]</td></tr>
<tr><td>12,000</td><td>3.70[1]</td></tr>
<tr><td>15,000</td><td>3.82[1]</td></tr>
<tr><td>20,000</td><td>4.0[1, 8]</td></tr>
<tr><td>50,000</td><td>4.3[8]</td></tr>
</table>

Dead-pressed if subjected to 25,000–30,000 psi[8, 19], dead-pressed >25,000–30,000 lb/in^2[9]</td></tr>
</table>

Density of MF as a function of loading pressure[9]:

Pressure (kpa)	Pressure (psi)	Density (g/cm^3)
20,685	3,000	3.0
68,450	10,000	3.6
137,900	20,000	4.0
344,750	50,000	4.3

ρ of MF as function of compacting pressure (specific surface = 754 cm^2/g)[12]:

Compacting pressure (MPa)	ρ (g/cm^3)	Compacting pressure (MPa)	ρ (g/cm^3)
~0	~1.25	~50	~3.55
~10	~2.75	~70	~3.7
~20	~3.1	~90	~3.8
~30	~3.3	~100	~3.9
~40	~3.45		

Heat of formation	941 kJ/kg (enthalpy of form.)[2], 226 cal/g[1, 4, 8], 221–226 kg cal/mol[9], −268 to −273 kJ/mol[12], 1,543 kJ/kg [Hg (g)] ($\Delta_f U°$, *Kast*, calorimetric bomb)[12], 1,660 kJ/kg ($\Delta_f U°$, *Wöhler*, calorimeter)[12], 65.7 kcal/g mol[23], 958 kJ/kg (energy of form.)[2]
Heat of combustion	938 cal/g[1, 4, 8, 9]

	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]	2,015	427 kcal/kg[5] 1,540 kJ/kg [Hg (g)][12] 1,803 kJ/kg [Hg (l)][12] 410 cal[13]	427 cal/g[1, 8, 9] 1,735[2] 410 cal/g[4] 368 cal/g[19]
T_{ex} [K]	4,394	4,400 °C (@ 4.0 g cm^{-3})[5] 3,530 °C[13]	4,450 °C[19]

<table>
<tr><td>$p_{C\text{-}J}$ [kbar]</td><td>246</td><td>220 (@ 4.0 g cm^{-3})[5]

264 (@ 4.41 g cm^{-3})[5]</td><td></td></tr>
<tr><td>VoD
[m s^{-1}]</td><td>4,976
(@ 4.42 g cm^{-3},
$\Delta_f H° = 268$ kJ mol^{-1})</td><td>6,910 (@ 4.0 g cm^{-3})[5]

6,000 (@ 4.41 g cm^{-3})[5]

5,000 (@ 4.0 g cm^{-3})[5]

5,400 (@ 4.2 g cm^{-3},
av. value from lit.)[4]</td><td>3,500 (@ 2.0 g cm^{-3},
pressed)[1, 9, 20]

4,250 (@ 3.0 g cm^{-3},
pressed)[1, 20]

4,200 (@ 3.0 g cm^{-3})[9]

5,000 (@ 4.0 g cm^{-3},
pressed)[1, 9, 20]

5,400 (@ 4.42 g cm^{-3})[4, 19]

3,260 (av. value @ 1.69 g cm^{-3},
25 °C, powder, thin-walled Pb
tubes, 12.5 mm diameter)[5]

3,100 (av. value @ 1.69 g cm^{-3},
–80 °C, powder, thin-walled Pb
tubes, 12.5 mm diameter)[5]

3,160 (av. value @ 1.69 g cm^{-3},
–180 °C, powder, thin-walled Pb
tubes, 12.5 mm diameter)[5]

Powder, thin-walled Pb
tubes, 12.5 mm diameter,
@ 1.69 g cm^{-3}[5]:

<table><tr><td>T = 25 °C</td><td>T = –80 °C</td><td>T –180 °C</td></tr><tr><td>3,320</td><td>3,060</td><td>3,150</td></tr><tr><td>3,200</td><td>2,960</td><td>3,170</td></tr><tr><td>3,260</td><td>3,270</td><td>–</td></tr><tr><td>3,260
(av.)</td><td>3,100
(av.)</td><td>3,160 (av.)</td></tr></table>
5,669 (calcd. value based on sand
test)[4]

5,400 (@ 4.17 g cm^{-3})[9]

5,050 (@ 4.0 g cm^{-3})[5]</td></tr>
</table>

			~4,000 (when loaded in commercial detonators and compressed under 3,000 lb/in^2, explodes from a spark)[13] 4,490 (@ 3.3 g cm^{-3}, detonator capsules, 8.7 mm internal diameter)[13] 16,500 ft/s (@ 4.00 g/mL)[17]
V_0 [L kg^{-1}]	215	315 mL/g[9] 311 dm^3 kg^{-1}[12] 314 (specific vol. = voL. of gaseous products @ 0 °C and 750 mm Hg)[13]	243 g cc[1] 315[3] 314[4] 315 (@ 0 °C and 760 mm Hg)[19]

Critical pressure of explosion initiation [GPa]	$P_{ult} = 0.20 \pm 0.01$[16], $p_{cr} = 0.20 \pm 0.01$ GPa[25]
Trauzl test [cm^3, % TNT]	51% TNT[1, 20], 37–50% TNT[8, 9], 110–150 cc (standard 10 g charge)[11], 51–54% TNT[4], 25.6 cc (2 g MF)[3], 51% TNT[12], 37–50% TNT[12], 23% PETN[13], 8.1 cc (1 g MF in no. 8 detonator capsule, compressed under reinforcing cap @ 3,400 lb/in^2, fired in small Trauzl block)[13], 150 cm^3 (10 g sample, sand tamping)[13], 8.1 cc (small Trauzl block test)[18]
Sand test [g]	27.3–59% TNT[9], 49–55% TNT[4], 22.5 g sand crushed (0.4 g sample, 1,700 g bomb)[4], 17.9–23.4 g sand crushed (0.4 g MF, 200 g bomb, cf. 48 g for TNT, that is, 27.3–59% TNT)[8], 37.3–48% TNT[12], 49% TNT[12], 23.4 g (200 g bomb)[20] No. 2 sand test bomb (No. 8 detonator capsule, pressed under reinforcing caps @ 3,400 lb/in^2, sand pulverized finer than 30 mesh)[13]:

Weight of charge (g)	Weight of sand pulverized (g)
0.10	3.1
0.20	6.5
0.40	17.0
0.60	27.5
0.80	38.0
1.00	48.4

Sand test bomb (weight of sand pulverized finer than 30 mesh (g))[13]:

Weight of charge (g)	Weight of sand pulverized (g)		
	MF	90:10 (fulminate:chlorate)	80:20 (fulminate:chlorate)
20,000	56.94	58.57	59.68
15,000	47.71	51.11	52.54
10,000	38.33	40.13	41.42
7,500	29.65	32.30	34.28
5,000	22.45	23.07	23.22
4,000	17.91	17.90	18.13
3,500	14.16	15.13	15.94
3,250	12.20	12.90	13.13
3,000	10.01	12.71	12.61
2,500	8.84	9.57	11.94
2,250	6.93	8.71	10.29
2,000	5.48	8.33	9.44

Sand crushing power (MF loaded into No. 6 detonator capsule, compressed @ 1000 lb/in^2)[13]:

Weight of charge (g)	Weight of sand crushed (g)
0.05	0.00
0.10	0.00
0.20	4.2
0.30	8.9
0.50	16.0
0.75	26.1
1.00	37.2

Sand test data from *Taylor* and *Rinkenbach*[13]:

Weight of MF (g)	Weight of sand crushed (g)
0.200	3.8
0.400	12.2
0.600	20.1
0.800	28.2
1.000	36.8

18.0 g (amount of sand crushed finer than 30 mesh, by base charge of MF)[18]

Initiating efficiency

Initiating efficiency: g required to give complete initiation of[1]

HE	Fulminate (g)
TNT	0.25
Tetryl	0.20
RDX	0.19
PETN	0.17

Max. reached @ $\rho = 3.2$ g cm^{-3}[12], dead-pressed @ $\rho = 3.6$ g cm^{-3}[12],

0.23 g, 0.24 g, 0.25 g, 0.26 g, 0.35 g, 0.36 g, 0.37 g for TNT[12]

Influence of compacting pressure and specific surface on initiation efficiency (acceptor = 0.35 g TNT compressed by 76.5 MPa, reinforcing cap)[12]:

Specific surface (cm^2/g)	Min. amount (g)	Compacting pressure (MPa)	Specific surface (cm^2/g)	Min. amount (g)	Compacting pressure (MPa)
5,570	~0.48	~2	8,990	~0.5	~46
	~0.43	~15	754	~0.18	~1
	~0.5	~17		–	~14
8,990	~0.29	~1		–	~29
	~0.29	~14		–	~44
	~0.31	~29		–	~58
	~0.42	~44		–	~59

Influence of ρ and specific surface on initiation efficiency (acceptor = 0.35 g TNT compressed by 76.5 MPa, reinforcing cap)[12]:

Specific surface (cm^2/g)	ρ (g/cm^3)	Min. amount (g)	Specific surface (cm^2/g)	ρ (g/cm^3)	Min. amount (g)
5,570	~2.2	~0.49	2,970	~3.75	~0.54
	~3.3	~0.47	754	~1.7	~0.19
	~3.4	~0.59		~2.8	~0.15
2,970	~2	~0.3		~3.4	~0.2
	~3.2	~0.295		~3.6	~0.305
	~3.5	~0.3		~3.7	~0.41
	~3.6	~0.41		~3.8	~0.48

Influence of reinforcing material (in brackets) on min. amount of MF required to detonate PETN with 50% probability[12]: 0.45 g (none), 0.24 g (Al), 0.18 g (Cu), 0.145 g (brass), 0.125 g (Fe)[12]

Minimum initiating charge (g) of MF for HEs (0.5 g HE in no. 8 detonator shell, primary added on top, both compressed under reinforcing capsule @ 3,400 lb/in^2)[13]: 0.150 g for pentryl[13], 0.225 g for PA[13], 0.240 g for TNT[13], 0.165 g for tetryl[13], 0.225 g for trinitroresorcinol[13], 0.165 g for trinitrobenzaldehyde[13], 0.175 g for tetranitroaniline[13], 0.165 g for hexanitrodiphenylamine[13], <0.4 g for pentryl if there is no reinforcing cap[13], 0.525 g for PA (Clark)[13]

Minimum initiating charge in g of MF for HEs (0.4 g HE in detonator capsule, pressing down, initiator added, covered with short reinforcing cap, pressing @ 2,000 atm/in^2)[13]: 0.26 g for TNT[13], 0.21 g for PA[13], 0.24 g for tetryl[13], 0.20 g for tetranitroaniline[13], 0.85 g for ammonium picrate[13], 0.30 g for guanidine picrate[13], 0.20 g for trinitroresorcinol[13]

0.29 g for tetryl[13], 0.30 g for PA[13], 0.36 g for TNT[13], 0.37 g for trinitroanisol[13], 0.40 g for trinitroxylene[13]

Minimum charges of MF required to initiate explosion of PETN (0.4 g PETN tamped down or pressed loosely into Cu capsules, 6.2 mm inside diameter, MF pressed loosely on top): 0.30 g gray MF[13], 0.30 g white MF[13], 0.330 g (gray MF, PETN compressed @ 2,000 kg/cm^2)[13], 0.340 g (white MF, PETN compressed @ 2,000 kg/cm^2)[13], dead-pressed (white MF, PETN compressed @ 2,000 kg/cm^2, 500 kg/cm^2 pressure on initiator)[13], dead-pressed (gray MF, PETN compressed @ 2,000 kg/cm^2, 500 kg/cm^2 pressure on initiator)[13]

<table>
<tr><td></td><td>0.24 g MF causes detonation of 0.4 g TNT in no. 6 detonator capsule when charge was confined by reinforcing cap[13]; 0.37 g MF when it was not confined[13]

No. of g of MF required for complete detonation of TNT: 0.25–0.36 g[9], 0.20–0.29 g for tetryl[9], 0.19 g for RDX[9], 0.17 g for PETN[9], 0.85 g for Explosive D[9]</td></tr>
<tr><td>Dead-pressing</td><td>Dead-pressed @ $\rho = 3.6$ g cm^{-3}[12], on pressing @ 25,000–30,000 lb/in^2[13]</td></tr>
<tr><td>5 s explosion T [°C]
1 s explosion T [°C]
0.1 s explosion T [°C]
Ignition T [°C]

5 s ignition T [°C]

Explosion T [°C]

<table>
<tr><td></td><td>Dependence of induction period on dilution, weight of fulminate = 0.02 g[26]:

<table><tr><td>T (°C)</td><td>induction period, pure fulminate (s)</td></tr><tr><td>193</td><td>5.7</td></tr><tr><td>183</td><td>14.4</td></tr></table></td></tr>
<tr><td>Flame sensitivity</td><td>1,000 MPa compacting pressure, 1 mm orifice diameter[12]:

<table><tr><td>Probability of initiation</td><td>Time in hydrogen flame (ms)</td></tr><tr><td>0</td><td>~2.5</td></tr><tr><td>30</td><td>~3.2</td></tr><tr><td>60</td><td>~3.8</td></tr><tr><td>70</td><td>~4.5</td></tr></table>
0 MPa compacting pressure, 3 mm orifice diameter[12]:

<table><tr><td>Probability of initiation</td><td>Time in hydrogen flame (ms)</td></tr><tr><td>0</td><td>~1.5</td></tr><tr><td>30</td><td>~1.5</td></tr><tr><td>60</td><td>~1.75</td></tr><tr><td>100</td><td>~1.7</td></tr></table></td></tr>
<tr><td>100 °C heat test [% mass loss]</td><td>Explodes in 16 h[1, 8]</td></tr>
<tr><td>75 °C int. heat loss test</td><td>0.18% loss in 48 h[1]</td></tr>
<tr><td>Vacuum stability test [cm^3/h]</td><td>@ 100 °C: explodes[1, 8]</td></tr>
</table>

Thermal stability

Effect of storage @ 50 °C (dry) on the purity (%) of MF[1]:

Months storage	Recrystallized lots				Uncrystallized lots	
	979	980	981	982	505.6–7/31	505.3–5/11
0	99.75	99.77	99.79	99.79	98.86	
4						98.7
6	99.38	99.45	99.54	99.47	95.95	98.7
8						97.4
9					94.5	
10						94.9
12	98.74	99.56	97.49	99.06	90.65	
13	98.26			98.79		
14	98.22					
15	97.52	99.30	99.30	98.19	83.76	
16	97.00		99.01	97.75		
17	95.70	98.66		96.69		
18	94.81	98.58	98.46	95.90	79.99	
23					74.52	
26					63.80	

Storage of 99.75% purity MF @ 50 °C for 24 months shows deterioration to 92%[8], ~7% mass loss within 45 days @ 75 °C[12], slow dec. @ 60 °C within 1 month[12], storage of 99.75% purity MF for 8 months @ 50 °C results in deterioration to 95% purity and after storage for 11 months deteriorates to 92% purity[19]

Time required for MF to lose ignition ability[12]: 3 years @ 35 °C, 9–10 months @ 50 °C, 10 days @ 80 °C[12], explodes in relatively short time @ T>85 °C[9]

Effect of storage @ 50 °C on purity of recryst. MF[12]:

Storage time (months)	Purity (%)
0	100
6	99
12	99
15	99
18	98

Effect of storage @ 50 °C on purity of nonrecryst. MF[12]:

Storage time (months)	Purity (%)
0	100
6	98
8	~98
12	~90
15	~85
18	80
23	~75
26	~65

Storage under water: purity decreases from 99.6–98.3% within 5 years[12], 6% decrease in brisance after 5 years[12]
Storage under sea water: 10% decrease in brisance after 2 years storage[12], 85% decrease in brisance after 3 years storage[12]

Completely inert after ~3 years @ 35 °C[13], completely inert after ~10 months @ 50 °C[13]

Deterioration of MF: approx. times of storage required to cause deterioration to 92% and 95%[9]:

Storage *T* (°C)	Time required to reduce purity to					
	95%			92%		
	Days	Months	Years	Days	Months	Years
80	0.5	–	–	1	–	–
50	–	8	–	–	11	–
30–35	–	–	1.7	–	–	5.8
20	–	–	7	–	–	9
10	–	–	8	–	–	10

MF will explode on storage @ *T* ~100 °C for ~16 h[20], prolonged exposure to tropical temperatures results in slow deterioration and loss in detonation ability[20], MF becomes inert on storage @ 35 °C for 3 years[20], MF becomes inert on storage @ 50 °C for 10 months[20], becomes completely insensitive after 9 days @ 80 °C (dry heating)[23], becomes insensitive under tropical hot–wet conditions @ 50 °C after 3–4 months[23]

<table>
<tr><td>Burn rate [mm/s]</td><td>0.05 (0.5 mm thick film)[12], 8.5 (2.75 mm thick film)[12], @ low pressure MF only burns[12]
linear and mass rates of burning @ 1 atm[22]: $u = 1.55$ cm/s[22], $m = 5.9$ g cm^{-2} s^{-1}[22]
burns without explosion if laid as a train in the open[23]</td></tr>
<tr><td>Solubility [g/mL]</td><td>Solubility in 100 g H_2O: 0.07 g @ 12 °C[1], 0.18 g @ 49 °C[1], 0.71 g/L in H_2O @ 12 °C[9], 1.74 g/L in H_2O @ 49 °C[9], 7.7 g/L H_2O @ 100 °C[9], soluble in NH_3, pyridine, ethanolamine[12], aq. NH_3, aq. KCN, pyridine[9, 19], slightly soluble in EtOH, acetone[12], very slightly soluble in hot Et_2O[12], insoluble in $CHCl_3$, glycol, benzene[12], 40 g/100 g diethanolamine @ 30 °C[12], 28 g/100 g triethanolamine @ 30 °C[12]

Solubility in H_2O[12, 13]:

<table><tr><td>T (°C)</td><td>Solubility (g/100 mL)</td></tr><tr><td>12</td><td>0.071</td></tr><tr><td>49</td><td>0.174</td></tr><tr><td>100</td><td>0.77</td></tr></table>
Soluble in EtOH, ammonium hydroxide (aq. NH_3) and aq. sodium thiosulfate soln.[17]</td></tr>
<tr><td>Hygroscopicity</td><td>0.02% @ 30 °C, 90% RH[1, 9], not hygroscopic[12, 17], however moisture reduces its sensitivity[17], practically nonhygroscopic[20], not hygroscopic[23]</td></tr>
<tr><td>Photosensitivity</td><td>Forms small amounts of Hg on exposure to light, or elevated T[1], dec. under UV light[12]

Photochemical sensitization of mercury fulminate[26]:

<table><tr><td>T (°C)</td><td>Normal induction period (s)</td><td>Induction period of exposed initiator (s)</td></tr><tr><td>197</td><td>7.0</td><td>6.3</td></tr><tr><td>181</td><td>22.2</td><td>19.7</td></tr></table></td></tr>
<tr><td>Compatibility</td><td>Reacts rapidly with aluminum and magnesium when dry, slowly with copper and zinc, brass and bronze[1, 9, 17] (reaction with metals is faster when moist) iron and steel are not affected[1, 9, 17], wet MF reacts immediately with Al and Mg[1], wet MF reacts rapidly with Cu, Zn, brass and bronze[1], wet MF does not affect iron or steel[1, 9], since MF forms small amounts of Hg on exposure to light or elevated temperature, it readily forms amalgams with Cu, brass and bronze meaning these metals have to be protectively coated if used with MF[1, 9], MF undergoes dec. in presence of aqueous solns. of carbonates, chlorides and others[1], MF detonates if steamed[17], reacts with conc. sulfuric acid[19], pure MF does not react with metals[19], standard grade MF contains ≤1% Hg which can cause slight erosion of Cu and its alloys[19],</td></tr>
</table>

<table>
<tr><td></td><td>reacts with conc. HCl[9], dry MF reacts vigorously with Al and Mg, slower with Cu, brass and bronze[20], wet MF reacts immediately with Cu, Zn, brass and bronze but does not react with Fe or steel[20], in presence of water it reacts with metals[23]</td></tr>
<tr><td>Stab sensitivity</td><td>Values from[1]
<table>
<tr><td rowspan="2">Density (g/cc)</td><td colspan="3">Firing point (in-oz)</td></tr>
<tr><td>0%</td><td>50%</td><td>100%</td></tr>
<tr><td>3.91</td><td>3.2</td><td>4.3</td><td>5.5</td></tr>
<tr><td>4.26</td><td>1.6</td><td>2.6</td><td>5.5</td></tr>
<tr><td>4.32</td><td>1.6</td><td>2.6</td><td>4.0</td></tr>
<tr><td>4.50</td><td>1.6</td><td>2.5</td><td>4.0</td></tr>
</table></td></tr>
<tr><td>Specific heat [cal/g/°C]</td><td>1.1[1]</td></tr>
<tr><td>Thermal conductivity [cal/s/cm/°C]</td><td>1×10^{-4}[1]</td></tr>
<tr><td>Laser sensitivity</td><td>MF can be successfully initiated using a UV excimer laser[21]:
<table>
<tr><td>Pressing force (kN)</td><td>Detonator type</td><td>Nominal wavelength (nm)</td><td>Function time (µs)</td><td>Source</td><td>Pulse duration (µs.)</td></tr>
<tr><td><100</td><td>Confined</td><td>249</td><td>3,500</td><td>Excimer laser</td><td>15</td></tr>
</table></td></tr>
<tr><td>Radiation sensitivity</td><td>MF irradiated at ambient T using 0.41 MeV $^{198}_{79}$Au γ-rays; volumes of gas produced measured during and after irradiation, amount of gas evolved as function of gamma dose [28]:
<table>
<tr><td>Gamma energy absorbed, 10^7 R</td><td>Gas evolved (mL/g) @ STP</td></tr>
<tr><td>1</td><td>0.2</td></tr>
<tr><td>2</td><td>0.8</td></tr>
<tr><td>2.5</td><td>2</td></tr>
<tr><td>3</td><td>> 4</td></tr>
</table></td></tr>
</table>

Minimum ignition energies of MF by light flashes, [a] = small quantity placed in a heated aluminum block and exploded within 30 s[28]:

Compound	Color	Thermal ignition T (°C)[a]	Electrical energy of flash, half-life 0.8 ms (J)	Light intensity (J/cm^2)
MF	light gray	190	200	1.65

Electric bridge wire

Bridge current and ignition time (I = ignition current (ampere), s = ignition time (1/1000 s), I^2s = (ignition current)^2 × (ignition time), crude MF)[24]:

I	2.0	1.6	1.3	1.0	0.8
s	6.3	8.6	11.6	20.1	37.8
I^2s	25.2	22.0	19.6	20.1	23.8

Bridge current and ignition time (I = ignition current (ampere), s = ignition time (1/1000 s), I^2s = (ignition current)^2 × (ignition time), powder MF)[24]:

I	2.0	1.6	1.3	1.0	0.8
s	2.8	4.0	6.1	10.5	18.7
I^2s	11.2	10.2	10.3	10.5	12.0

Bridge current and ignition time (I = ignition current (ampere), s = ignition time (1/1000 s), I^2s = (ignition current)^2 × (ignition time), white MF)[24]:

I	2.0	1.6	1.3	1.0	0.8
s	2.9	3.7	5.2	7.2	15.4
I^2s	11.6	9.8	8.8	7.2	9.9

	Mercury fulminate[6]	**Mercury fulminate**[24]
Chemical formula	$C_2N_2O_2Hg$	$C_2N_2O_2Hg$
Molecular weight [g mol^{-1}]	284.63	284.63
Crystal system	Orthorhombic	
Space group	*C m c a* (no. 64)	
a [Å]	5.3549(2)	7.71

b [Å]	10.4585(5)	5.48
c [Å]	7.5579(4)	10.43
α [°]	90	
β [°]	90	
γ [°]	90	
V [Å^3]	423.27(3)	
Z	4	4
ρ_{calc} [g cm^{-3}]	4.467	
T [K]	100	

* Yellow-white silky crystals: dissolving MF in boiling H_2O followed by decanting and cooling liquid[12]

White crystals: recrystallization from aqueous NH_3 without neutralization[12]

Pyramidal crystals: recrystallization from NH_3/H_2O/EtOH[12]

Lustrous flakes: pouring a pyridine MF soln. into Et_2O[12]

Large thin white rhomboids: brown or white MF dissolved in hot pyridine then left to cool[12]

Crystallization of MF from water produces a hydrate: $Hg(CNO)_2 \cdot {}^1/_2\ H_2O$[9], anhydrous MF is recrystallized form EtOH (usually truncated octahedral crystals)[8]

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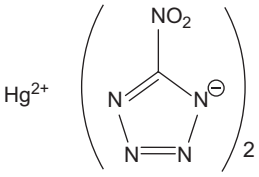
Mercury nitrotetrazolate

Name [German, acronym]: Mercuric nitrotetrazole, [Quecksilbernitrotetrazolat]
Main (potential) use: Investigated as possible component of detonant/stab sensitive composition

Structural formula:



	Mercury nitrotetrazolate		
Formula	$C_2HgN_{10}O_4$		
Molecular mass [g mol^{-1}]	428.68		
Appearance at RT	Heavy, granular crystal powder[2]		
IS [J]	Ball and disc: 6 cm, 3/50 fires[1]; 5 cm, 0/50 fires[1]		
FS [N]	Emery friction (A polymorph): 5 ft/s, 4/10 fires[1]; 4 ft/s, 2/10 fires[1]; 3 ft/s, 0/10 fires[1]		
ESD [J]	Minimum electrostatic energy to fire metal/metal electrodes = 270 µJ (partials)[1]		
N [%]	32.7		
$\Omega(CO_2)$ [%]			
$T_{m.p.}$ [°C]			
$T_{dec.}$ [°C]			
ρ [g cm^{-3}]			
Heat of formation			
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]			
T_{ex} [K]			
$p_{C\text{-}J}$ [kbar]			
VoD [m s^{-1}]			

V_0 [L kg^{-1}]			
Initiating efficiency	0.006 g for tetryl[2]		
5 s explosion *T* [°C] Ignition *T* [°C]	190 (@ 5 °C/min)[1], ~215 (detonates)[2]		
Vacuum stability test [cm^3/h]	0.06% mass loss @ 100 °C, 0.2 mm Hg vacuum for 1 week (A polymorph)[1]		
Solubility [g/mL]	Difficultly soluble in water but more soluble in water than the Ag salt[2]		
Compatibility	Less compatible with sulfur-containing rubbers and Al than the corresponding silver salt is[1], not attacked by nitric acid[2]		
Stab sensitivity	Insensitive[1]		
ERDET test [wt. found to detonate RDX in an ERDET]	30 mg [1]		
Dead pressing	Performance improves over 77 MN/m^2[1]		

Only one type of mercury nitrotetrazolate was found using X-ray powder photography patterns: A[1]

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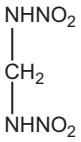
Methylene dinitramine

Name [German, acronym]: Methylene dinitramine, *N*,*N*-dinitromethanediamine, [MEDINA]
Main (potential) use: unknown
Structural formula:



	MEDINA		
Formula	$CH_4N_4O_4$		
Molecular mass [g mol^{-1}]	136.17		
Appearance at RT	10–11 in (P.A.)[1], 14–21 cm (B.M.)[1]		
IS [J]			
FS [N]			
ESD [J]			
N [%]	41.18		
$\Omega(CO_2)$ [%]	0.0		
$T_{m.p.}$ [°C]	105–106[1], 104[1], 103.5–104.5[1]		
$T_{phase\ transition}$ [°C]	Phase I from soln.[1], phase II (unstable from melt)[1]		
$T_{dec.}$ [°C]			
ρ [g cm^{-3}]			
Heat of formation	–13.84 kcal/mol[1]		
Heat of combustion	–230.2 kcal/mol[1], –216.35 kcal/mol (@ 25 °C)[1]		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]			
T_{ex} [K]			
$p_{C\text{-}J}$ [kbar]			

VoD [m s^{-1}]		8,500 (@ 1.68 g cm^{-3})[2] 8,700 (no ρ given)[1]	
V_0 [L kg^{-1}]			
Trauzl test	681–727 cc (10 g sample)[1], 188–210% TNT[2], 572[3]		
Sand test [sand crushed g]	71.9 (RDX = 58–61 g)[1], 127–131% TNT[2]		
Ballistic mortar test (% power TNT)	198[1], 154–158[2]		
5 s explosion T [°C]	300–330[1]		
100 °C heat test [% mass loss] International heat test	1.13–3.89% wt. loss after 72 h @ 80 °C[1] 2.77–6.54% wt. loss after 72 h @ 85 °C[1] 0.66% wt. loss after 4 h @ 75 °C[1] 1.47–2.24% wt. loss after 72 h @ 75 °C[1]		
Vacuum stability test [cm^3/h]	1.92 mg/g gas evolved after 40 h (T not specified)[1] 0.89–0.98 mL/g/40 h (T not specified)[1]		

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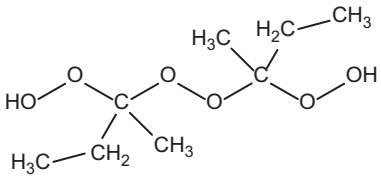
Methyl ethyl ketone peroxide

Name [German, acronym]: 2,2′-Peroxydi(butane-2-peroxol), 2-butanone peroxide, ethyl methyl ketone peroxide, 2-[(2-hydroperoxybutan-2-yl)peroxy]butane-2-peroxol, 2-hydroperoxy-2-(2-hydroperoxybutan-2-ylperoxy)butane [MEKP]*

Main (potential) use: HME

Structural formula:



	MEKP		
Formula	$C_8H_{18}O_6$		
Molecular mass [g mol^{-1}]	210.23		
Appearance at RT	Liquid (9% active oxygen (AO))[1], liquid (11% AO)[1],		
IS [J]	35 mJ[3]		
N [%]	0.0		
Ω(CO_2) [%]	−144.60		
$T_{m.p.}$ [°C]	110[3]		
$T_{dec.}$ [°C]			
ρ [g cm^{-3}]	1.17[3]		
Heat of formation			
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{ex}U^{o}$ [kJ kg^{-1}]			
T_{ex} [K]			
$p_{C\text{-}J}$ [kbar]			
VoD [m s^{-1}]			
V_0 [L kg^{-1}]			

<table>
<tr><td>Ballistic mortar test</td><td>MEKP (9% AO) = 18.0 weight strength of TNT[1]
MEKP (11% AO) = 26.0 weight strength of TNT[1]</td></tr>
<tr><td>Koenen and Ide BAM test</td><td>Values from[1]
<table>
<tr><th>Parameter</th><th>MEKP (9% AO)</th><th>MEKP (11% AO)</th></tr>
<tr><td>Orifice diameter, d (mm)</td><td>1.0</td><td>6.0</td></tr>
<tr><td>t_1 (s)</td><td>18.0</td><td>14.0</td></tr>
<tr><td>t_2 (s)</td><td>10.0</td><td>7.0</td></tr>
<tr><td>Time function, $\sqrt{t1/d + t2/d}$</td><td>14.2</td><td>2.68</td></tr>
<tr><td>Remarks</td><td>Steel case broke into 4 pieces</td><td>Steel case broke into 4 pieces</td></tr>
</table></td></tr>
<tr><td>Heavy confinement cap tests</td><td>Values from[1]:
<table>
<tr><th>Test sample</th><th>Average height (m)</th><th>Rel. height (% NM)</th><th>Rel. height (% TNT)</th></tr>
<tr><td>MEKP (9% AO)</td><td>6.1</td><td>25.0</td><td>26.2</td></tr>
<tr><td>MEKP (11% AO)</td><td>7.8</td><td>32.7</td><td>34.2</td></tr>
</table></td></tr>
<tr><td>Card gap test</td><td>Values from[1]
<table>
<tr><th rowspan="2">Test sample</th><th colspan="4">Results</th></tr>
<tr><th>Gap value (cm)</th><th>Velocity (m/s)</th><th>Acceptor and plate damage</th><th>Nature of reaction</th></tr>
<tr><td>MEKP (9% AO)</td><td>0</td><td>4,320, 1,420‡</td><td>5.0 cm length of acceptor at top, no plate damage</td><td>Only small part of sample reacted, incomplete reaction</td></tr>
<tr><td>MEKP (11% AO)</td><td>0</td><td>1,973, 1,019‡</td><td>10.0 cm length of acceptor at top, no plate damage</td><td>Only small part of sample reacted, incomplete reaction</td></tr>
</table>
‡ The velocity to which the shock wave decays in each test</td></tr>
</table>

<table>
<tr><td>DDT test</td><td>Values from[1]:
<table>
<tr><th>Test sample</th><th>No. of fragments</th><th>Remarks</th></tr>
<tr><td>MEKP (9% AO)</td><td>0</td><td>Pipe slightly bulged at one end, 1 cap ruptured into 2 pieces</td></tr>
<tr><td>MEKP (11% AO)</td><td>0</td><td>Pipe split open, both caps remain undamaged</td></tr>
</table></td></tr>
<tr><td>Bubble energies</td><td>MEKP (9% AO) = 3.7% TNT[1], MEKP (11% AO) = 6.5% TNT[1]</td></tr>
<tr><td>5 s explosion
T [°C]
Explosion T [°C]</td><td>123 (MEKP (9% AO), pipe damage: thermocouple plugs blew out, holes enlarged and pipe distorted)[1], 93 (MEKP (11% AO), sample found to be incompatible with the configuration, pipe damage: 1 cap off, pipe split-opened up to 22 cm)[1]</td></tr>
<tr><td>Deflagration properties</td><td>5 g sample, Pb_3O_4 (70 wt.%) – Si (30 wt.%) igniter, firing with a nichrome wire or fusehead, brass rupture disk of 0.15 mm thickness[2]: MEKP purity = 56.6 wt.%, 10.30% AO, liquid, amount of igniter giving the apparent max. rate of pressure rise = 1 g, Δ_{time} = 97 ms @ 100–300 psi, Δ_{time} = 42 ms @ 300–500 psi[2]</td></tr>
</table>

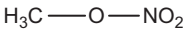
** MEKP with 9% or 11% AO are known*

[1] V. K. Mohan, K. R. Becker, J. E. Hay, *J. Hazard. Mater.*, **1982**, *5*, 197–220.
[2] M. Tamura, H. Ishida, M. Itoh, T. Yoshida, M. Watanabe, K. Muranaga, T. Abe, S. Morisaki, *J. Hazard. Mater.*, **1987**, *17*, 89–98.
[3] T. M. Klapötke, T. Wloka, *Peroxide Explosives*, ch. 29 in *Patai's Chemistry of Functional Groups*, John Wiley and Sons Ltd., **2014**, pp. 1–28.

Methyl nitrate

Name [German, acronym]: Methyl nitrate [methylnitrat]
Main (potential) use: Not of practical use due to its physical properties[1], mixed with H_2O_2 or N_2O_4 is used as liquid explosive or propellant[7], gas-generating agent in airbags[7]

Structural formula:



	Methyl nitrate		
Formula	CH_3NO_3		
Molecular mass [g mol^{-1}]	77.04		
Appearance at RT	Colorless liquid[1], colorless oily liquid with slight fragrant odor[7]		
IS [J]	40 mm (2 kg mass; is therefore less sensitive than NG)[7]		
ESD [J]	Explodes on heating @ 250–300 °C in a closed system on exposure to spark[7]		
N [%]	18.18		
$\Omega(CO_2)$ [%]	−10.4		
$T_{m.p.}$ [°C]	−83[10]		
$T_{b.p.}$ [°C]	65–66[1, 7], 5 (@ 50 mm)[1], 66 (@ 760 mm)[1], 338.0 K[2], 65[7], 64.6[10]		
$T_{dec.}$ [°C]	Vapors explode on heating to ~150[1]		
ρ [g cm^{-3}]	sp. gr. = 1.2322 (@ 5 °C)[1], sp. gr. = 1.2167 (@ 15 °C)[1], sp. gr. = 1.2032 (@ 25 °C)[1], sp. gr. = 1.21[7], 1.2075[10]		
Heat of formation	−122 kJ/mol ($\Delta_f H°(g)$)[2], $\Delta H_{f,r}$ = −1.91 MJ/kg[5], −155.8 kJ/mol (enthalpy of form., exptl.)[8], −187.5 kJ/mol (enthalpy of form., calcd., emp.)[8], −28.8 kcal/mol ($\Delta H_f(g)°$, calcd., ccCA-P)[9], −30.5 kcal/mol ($\Delta H_f(g)°$, calcd., ccCA-S3)[9], −29.7 kcal/mol ($\Delta H_f(g)°$, calcd., ccCA-PS3)[9], −29.6 kcal/mol ($\Delta H_f(g)°$, calcd., G3)[9], −27.3 kcal/mol ($\Delta H_f(g)°$, calcd., G3(MP2))[9], −29.2 ± 0.3 kcal/mol ($\Delta H_f(g)°$, exptl.)[9]		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.

<table>
<tr><td>$-\Delta_{ex}U°$ [kJ kg^{-1}]</td><td></td><td>6.29 MJ/kg (calcd., SD method)[3]

6.12 MJ/kg (heat of explosion)[5]

6,732.1–6,744.15[7]</td><td></td></tr>
<tr><td>T_{ex} [K]</td><td></td><td>4,290 (calcd., SD method)[3]</td><td></td></tr>
<tr><td>$p_{C\text{-}J}$ [kbar]</td><td></td><td></td><td></td></tr>
<tr><td>VoD [m s^{-1}]</td><td></td><td></td><td>VoD measured in tubes of such small diameter that max VoD was not obtained[1]:

<table><tr><td>Tube of</td><td>Internal diameter (mm)</td><td>External diameter (mm)</td><td>VoD (m/s)</td></tr><tr><td>Rubber, canvas covered</td><td>5</td><td>12</td><td>1,616</td></tr><tr><td>Glass</td><td>3</td><td>12</td><td>2,482</td></tr><tr><td>Glass</td><td>3</td><td>7</td><td>2,191</td></tr><tr><td>Glass</td><td>5</td><td>7</td><td>1,890</td></tr><tr><td>Britannia metal</td><td>3</td><td>12.6</td><td>1230</td></tr><tr><td>Steel</td><td>3</td><td>15</td><td>2,084</td></tr><tr><td>Steel</td><td>3</td><td>15</td><td>2,094</td></tr></table>
6,818 (@ 1.22 g cm^{-3}, D_i) (D_i = ideal detonation velocity)[3]

5,938 (@ 1.22 g cm^{-3}, D_f) (D_f = detonation velocity for critical detonation diameter)[3]

~8,000 in tube with 30–40 mm diameter, no ρ specified[7]

~1,500 in tube with small diameter, no ρ specified, but >6,000 in a large tube[7]</td></tr>
<tr><td>V_0 [L kg^{-1}]</td><td></td><td></td><td></td></tr>
<tr><td></td><td colspan="3"></td></tr>
<tr><td>Critical diameter [cm]</td><td colspan="3">2.4 mm[3]</td></tr>
</table>

<table>
<tr><td>Trauzl test [cm^3, % TNT]</td><td>615 cc (10 g sample, H_2O tamping c.f. 600 cc by 10 g NG)[1], 610[6]</td></tr>
<tr><td>Small lead block test</td><td>24.5 mm (100 g sample, under slight confinement in shell of sheet Pb 1 mm thick, tamped with thin cork plates, cf. 30 mm by nitroglycol and 18.5 mm by NG)[1]</td></tr>
<tr><td>Viscosity</td><td>less viscos than H_2O[1, 7]</td></tr>
<tr><td>Burn rate [mm/s]</td><td>0.143 g cm^{-2}s^{-1} @ 1 atm.[4], 4 times faster than that of NG[7], 0.12 cm/s in glass tube and burns slowly @ 0.15 MPa[7], @ pressures >0.4 MPa combustion escalates into detonation[7]

Dependence of burning rate on pressure ($MeONO_2$, ρ_{max} = 1.21 g/cm^3)[4]:

<table>
<tr><td rowspan="2">$\delta = \rho/\rho_{max}$</td><td colspan="3">Coefficients in formulae
m(gm cm^{-2} s^{-1}) = a + b p$^v_{atm}$</td><td rowspan="2">Pressure (atm)</td></tr>
<tr><td>a</td><td>B</td><td>v</td></tr>
<tr><td rowspan="2">1.0</td><td>0.01</td><td>0.133</td><td>1.0</td><td>0.175–2.0</td></tr>
<tr><td>–</td><td>0.141</td><td>0.99</td><td>0.5–1.5</td></tr>
</table>
</td></tr>
<tr><td>Solubility [g/mL]</td><td>Miscible with any alcohols[7], 3.85 g/100 mL H_2O @ 25 °C[7], $MeONO_2$ is good at dissolving cotton and high-nitrogen cellulose[7], soluble in EtOH, Et_2O[10], slightly soluble in water[10]</td></tr>
<tr><td>Heat capacity [J/mol K]</td><td>C_p (liq.) = 157.19 (@ 298 K, constant pressure)[2]</td></tr>
<tr><td>$\Delta_{vap}H°$ [kJ/mol]</td><td>34.10[2]</td></tr>
<tr><td>Flame sensitivity</td><td>Vapor is flammable and explodes on heating to 150 °C[7], heating @ 250–300 °C in closed system explodes on exposure to spark or UV radiation[7]</td></tr>
<tr><td>Radiation sensitivity</td><td>Explodes on heating @ 250–300 °C in a closed system on exposure to UV radiation[7]</td></tr>
<tr><td>n_D</td><td>1.3748[10]</td></tr>
</table>

[1] T. L. Davis, *The Chemistry of Powder and Explosives*, *vol. 2*, **1943**, John Wiley and Sons Inc., New York.

[2] P. J. Lindstrom,W. G. Mallard, *NIST Chemistry WebBook*, NIST Standard Reference Database, National Institute of Standards and Technology, Gaithersburg, USA, webbook.nist.gov.

[3] G. D. Kozak, *Combust. Expl. Shock Waves*, **1998**, *34*, 581–586.

[4] N. N. Bakhman, A. F. Belyaev, *Combustion of Heterogeneous Condensed Systems*, translated from *Gorenje Geterogennykh Kondensirovannykh Sistem*, Institute of Chemical Physics, Academy of Science, U.S.S.R. Moscow, Nauka Publication (1967) by C. A. J. Elphinston, M. Goyer, I. C. Graham, G. A. Heath, G. R. Ramsden, R.P.E. Translation No. 19, Ministry of Technology, London, November **1967**.

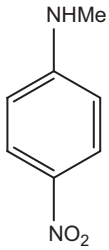
[5] N. Kubota, *Propellants and Explosives – Thermochemical Aspects of Combustion*, Wiley-VCH, **2002**.
[6] M. Jafari, M. Kamalvand, M. H. Keshavarz, S. Farrashi, *ZAAC*, **2015**, *641*, 2446–2451.
[7] J. Liu, *Nitrate Esters Chemistry and Technology*, Springer, **2019**.
[8] B. Nazari, M. H. Keshavarz, M. Hamadanian, S. Mosavi, A. R. Ghaedsharafi, H. R. Pouretedal, *Fluid Phase Equilibria,* **2016**, *408*, 248–258.
[9] K. R. Jorgensen, G. A. Oyedepo, A. K. Wilson, *J. Hazard. Mater.*, **2011**, *186*, 583–589.
[10] *CRC Handbook of Chemistry and Physics*, *Internet version 2005*, D. R. Lide (Editor-in-Chief), CRC Press, Boca Raton, FL, **2005**.

N-Methyl-4-nitroaniline

Name [German, acronym]: *N*-Methyl-*p*-nitro aniline, 4-(methylamino) nitrobenzene, 4-nitro-*N*-methylaniline, methyl(4-nitrophenyl)amine, *p*-nitro-*N*-methylaniline, *N*-methyl-4-nitro-benzenamine [*N*-methyl-4-nitroanilin, MNA]

Main (potential) use: Lowers mpt. of energetic materials in synthesis of insensitive explosives[1], stabilizer in double-base and minimum smoke propellants[1, 2], component of PAX-21[2]

Structural formula:



	MNA		
Formula	$C_7H_8N_2O_2$		
Molecular mass [g mol^{-1}]	152.15		
Appearance at RT	Yellow crystalline plates[4]		
N [%]	18.41		
$\Omega(CO_2)$ [%]	−168.26		
$T_{m.p.}$ [°C]	423.15 K[1]		
$T_{b.p.}$ [°C]	527 K[1]		
$T_{dec.}$ [°C]			
ρ [g cm^{-3}]	1.26[1]		
Heat of formation			
Heat of combustion	$\Delta_c H°$ (solid) = −3,867 kJ/mol[3]		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]			
T_{ex} [K]			

$p_{C\text{-}J}$ [kbar]			
VoD [m s^{-1}]			
V_0 [L kg^{-1}]			

Critical temperature [°C]	748 K[1]
Critical pressure	41.7 bar[1]
Solubility [g/mL]	1.17 mg/L @ 298.15 K[1] Solubility in H_2O in presence of NaCl or $CaCl_2$ @ different T[1, 2]:

Solvent	Solubility (mL/L)		
	@ 298.15 K	@ 308.15 K	@ 318.15 K
H_2O	85.42 ± 0.85	111.51 ± 1.12	141.93 ± 1.42
1% NaCl	79.49 ± 0.80	96.65 ± 0.97	128.17 ± 1.28
1% $CaCl_2$	82.82 ± 0.83	104.99 ± 1.05	134.81 ± 1.35

Log K_{ow}	2.1028 ± 0.0209 @ 298.15 K[1, 2], 1.9846 ± 0.0305 @ 308.15 K[1, 2], 1.9377 ± 0.0146 @ 318.15 K[1, 2]
Enthalpy of fusion [kJ/mol]	18.85[1]

	MNA[4]
Chemical formula	$C_7H_8N_2O_2$
Molecular weight [g mol^{-1}]	152.15
Crystal system	Monoclinic
Space group	$P2_1/n$ (no. 14)
a [Å]	9.9223(8)
b [Å]	6.8557(5)
c [Å]	10.7606(9)
α [°]	90
β [°]	103.304(8)
γ [°]	90
V [Å^3]	712.34(10)
Z	4

ρ_{calc} [g cm^{-3}]	1.419
T [K]	150

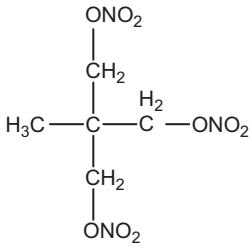
[1] D. S. Viswanath, T. K. Ghosh, V. M. Boddu, *N-Methyl-4-Nitroaniline (MNA)*, Ch. 7 in *Emerging Energetic Materials: Synthesis, Physicochemical, and Detonation Properties*, Springer, **2018**.
[2] V. M. Boddu, K. Abburi, S. W. Maloney, R. Damavarapu, *J. Hazard. Mater.*, **2008**, *155*, 288–294.
[3] W. E. Garner, C. L. Abernethy, *Proc. Roy. Soc. London A*, **1921**, 213–235.
[4] K. Gazda, Z. Daszkiewicz, E. Kozubek, K. Ejsmont, B. Zarychta, *Cryst. Growth Des.*, **2014**, *14*, 5737–5748.

Metriol trinitrate

Name [German, acronym]: 1,1,1-Trimethylolethane trinitrate, nitropentaglycerin, trimethylolethane trinitrate, ethane-1,1,1-tris(hydroxymethyl) trinitrate, pentaglycerol trinitrate, nitrometriol [TMETN, MtrT, MTN]

Main (potential) use: Erosion-reducing additive in propellants[1], component of commercial explosives[1], ingredient of rocket and double-base propellants[3], suggested as possible replacement for NG[8], component of smokeless (double-base) powders in the WW-II[8], nitrate-ester plasticizer[13]

Structural formula:



	Metriol trinitrate
Formula	$C_5H_9N_3O_9$
Molecular mass [g mol^{-1}]	255.15
Appearance at RT	Slightly turbid viscos oil[1], slightly turbid oil[3], liquid @ RT[8]
IS [J]	4 cm (2 kg mass, B.M.)[1, 4], 20 in (P.A.)[3, 4], 0.59 kg/m (50% detonations)[6], 47 cm (1 lb mass, B.M., 20 mg sample)[7], similar to that of tetryl[8], 47 cm (2 kg mass, 20 mg sample, B.M.)[3], 4 cm (1 lb mass, 20 mg sample, B.M.)[3]
FS [N]	Explodes with steel shoe (friction pendulum test)[1, 3], explodes with fiber shoe (friction pendulum test)[1]
N [%]	16.41
$\Omega(CO_2)$ [%]	−34.5
$T_{m.p.}$ [°C]	−3[1, 3, 4, 7], 51[8]
$T_{glass\ transition}$ [°C]	−63.5[11], −45.2 (midpoint, DSC @ 10 °C/min, with 50% polyNIMMO)[13]
$T_{b.p.}$ [°C]	182 (apparent b.p., corresponds to temperature at which dec. is vigorous enough to resemble boiling)[1]

$T_{dec.}$ [°C]	177.7 (onset), 198.6 (peak max), 219.0 (end T) (DSC @ 10.0 K/min, pinhole cover)[10]		
ρ [g cm^{-3}]	1.47 (@ 22 °C)[1, 4, 7], sp. gr. = 1.4685 (@ 20/4°)[6, 8], 1.48–1.50 (after being fused it solidifies to a solid of this ρ)[8], 1.47 (liquid)[3], 1.49[11]		
Heat of formation	−450.2 kJ/mol[2], −422 cal/g (@ C^v)[1, 4], −446 cal/g (@ C^p)[1, 4], −1,666 kJ/kg (ΔH_f, ICT thermochemical database)[9], −425.0 kJ/mol (enthalpy of form., exptl.)[12], −426.6 kJ/mol (enthalpy of form., calcd., emp.)[12], −434.5 kJ/mol (enthalpy of form., calcd., S-D method)[12]		
Heat of combustion	−2,642 cal/g (@ C^v, H_2O (l))[1, 4, 5, 7], 674 kcal/mol[4], 2,642 cal/g[3]		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]		1,270 kcal/kg[8] 5,053 (calcd., ICT-code)[9]	
T_{ex} [K]		3,497 (calcd., ICT-code)[9]	
$p_{C\text{-}J}$ [kbar]		140.9 MPa (calcd., ICT-code)[9]	
VoD [m s^{-1}]		7,300 (@ 1.640 g cm^{-3}, calcd., K-J)[10]	6,750 (@ 1.39 g cm^{-3}, nonconfined nitrometriol cartridges, 30 mm diameter)[8] 7,040 (@ 1.48 g cm^{-3}, nonconfined nitrometriol cartridges, 30 mm diameter)[8] 7,060 (@ 1.50 g cm^{-3}, nonconfined nitrometriol cartridges, 30 mm diameter)[8]
V_0 [L kg^{-1}]			
Trauzl test [cm^3, % TNT]	140[1, 3, 4], ~85% penthrite[8], ~115% PA[8]		
Sand test [g]	43.7 (200 g bomb)[1, 3, 4, 7], 91% TNT[1, 4]		

<table>
<tr><td>Ballistic mortar test</td><td>136% TNT[1, 3, 4]</td></tr>
<tr><td>5 s explosion T [°C]
Deflagration T [°C]</td><td>235[1, 3, 4], 235 (ignites)[3, 5, 7]
188 (@ 2 °C/min, with 50% polyNIMMO)[13]</td></tr>
<tr><td>100 °C heat test
[% mass loss]</td><td>2.5 in first 48 h[1, 3, 4, 7], 1.8 in s 48 h[1, 3, 4, 7], no explosions in first 100 h[1, 3, 4, 7]</td></tr>
<tr><td>Thermal stability</td><td>Nonisothermal TG data, β = °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.[10]:
<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>158.8</td><td>178.3</td><td>208.9</td><td>169.3</td></tr>
<tr><td>7.0</td><td>161.8</td><td>183.4</td><td>216.7</td><td></td></tr>
<tr><td>10.0</td><td>167.0</td><td>188.3</td><td>222.5</td><td></td></tr>
<tr><td>15.0</td><td>177.1</td><td>196.0</td><td>225.0</td><td></td></tr>
</table></td></tr>
<tr><td>Vacuum stability test
[cm^3/h]</td><td>1.9 cm^3/40 h (@ 100 °C)[1, 3, 4]</td></tr>
<tr><td>Volatility</td><td>24 mg/cm^2 lost in 1 hour @ 60 °C[1, 3, 4]</td></tr>
<tr><td>Solubility [g/mL]</td><td>Practically insoluble in water[1], soluble in EtOH and many common organic solvents[1], <0.015 g/100 g H_2O @ 25 °C[1, 3], <0.015 g/100 g H_2O @ 60 °C[3], 0.516 g/L H_2O @ 19 °C[8], 0.685 g/L H_2O @ 36 °C[8]</td></tr>
<tr><td>Hygroscopicity</td><td>0.07% @ 25 °C with 90% RH[1], 0.14% @ 25 °C with 100% RH[1], 0.07% @ 30 °C, 90% RH[3]</td></tr>
<tr><td>Compatibility</td><td>Acid bath hydrolysis: 10 days @ 22 °C, 0.018% hydrolysis[1, 3], 5 days @ 60 °C, 0.115% hydrolysis[1, 3]</td></tr>
<tr><td>$\Delta H_{dec.}$ [J/g]</td><td>323.0 (heat release, value not reliable due to evaporation at low heating rates)[10]</td></tr>
<tr><td>Refractive index</td><td>n^D_{25} = 1.4752[1, 3]</td></tr>
<tr><td>Dutch test</td><td>1.50% (105 °C, 72 h, ≤2%, with 50% polyNIMMO)[13]</td></tr>
<tr><td>Viscosity [Pa•s]</td><td>5.12 (with 50% polyNIMMO)[13]</td></tr>
</table>

[1] *Military Explosives*, Department of the Army Technical Manual, TM 9-1300-214, Headquarters, Department of the Army, September **1984**.

[2] *NIST Chemistry WebBook*, NIST Standard Reference Database, P. J. Linstrom, W. G. Mallard (eds.), National Institute of Standards and Technology, Gaithersburg, USA: www.webbook.nist.gov/chemistry/

[3] *AMC Pamphlet Engineering Design Handbook: Explosive Series of Properties of Explosives of Military Interest*, Headquarters, US Army Materiel Command, January **1971**.

[4] S. M. Kaye, *Encyclopedia of Explosives and Related Items*, *vol. 8*, US Army Research and Development Command, TACOM, Picatinny Arsenal, USA, **1978**.

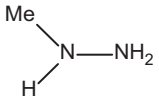
[5] B. T. Fedoroff, O. E. Sheffield, *Encyclopedia of Explosives and Related Items*, *vol. 4*, US Army Research and Development Command, TACOM, Picatinny Arsenal, USA, **1969**.
[6] B. T. Fedoroff, O. E. Sheffield, *Encyclopedia of Explosives and Related Items*, *vol. 6*, US Army Research and Development Command, TACOM, Picatinny Arsenal, USA, **1974**.
[7] F. J. Pisacare, *1,2,4-Butanetriol: Analysis and Synthesis*, NSWC TR 82-380, NSWC, 8th December **1982**.
[8] T. Urbański, Ch. 8 in *Chemistry and Technology of Explosives*, *vol. II*, **1965**, Pergamon Press, Oxford.
[9] F. Volk, H. Bathelt, *Propellants, Explosives, Pyrotechnics*, **2002**, *27*, 136–141.
[10] Q.-L. Yan, M. Künzel, S. Zeman, R. Svoboda, M. Bartošková, *Thermochim. Acta*, **2013**, *566*, 137–148.
[11] M. F. Lemos, M. A. Bohn, *The Effect of Plasticizers on the Glass-to-Rubber Behavior of Desmophen® 2200 Based Elastomers Used for Composite Propellants*, ICT **2015**, Karlsruhe, Germany, pp. 22-1–22-26.
[12] B. Nazari, M. H. Keshavarz, M. Hamadanian, S. Mosavi, A. R. Ghaedsharafi, H. R. Pouretedal, *Fluid Phase Equilibria,* **2016**, *408*, 248–258.
[13] D. Drees, D. Löffel, A. Messmer, K. Schmid, *Propellants, Explosives, Pyrotechnics*, **1999**, *24*, 159–162.

Monomethylhydrazine

Name [German, acronym]: Methylhydrazine, hydrazomethane, 1-methylhydrazine, [monomethylhydrazin, MMH]

Main (potential) use: Component of hypergolic systems[1]

Structural formula:



	MMH		
Formula	CH_6N_2		
Molecular mass [g mol^{-1}]	46.07		
Appearance at RT	Colorless liquid		
IS [J]	Stable to impact[2]		
FS [N]	Stable to friction[2]		
ESD [J]	MMH vapors within flammable limits can be exploded by a spark or flame[2]		
N [%]	60.80		
$\Omega(CO_2)$ [%]	−173.65		
$T_{m.p.}$ [°C]	−52[1], (−52.4 freezing point[2])		
$T_{b.p.}$ [°C]	87[1], 87.5[2]		
$T_{dec.}$ [°C]	1,828 K (adiabatic dec. *T*, calcd. CHEETAH)[3]		
ρ [g cm^{-3}]	0.874[1], 0.8743 @ 25 °C[2]		
Heat of formation	54.18 kJ/mol (enthalpy of form.)[1], 12.7 kcal/mol[2], 54.14 kJ/mol ($\Delta_f H°$ liq., calorimetry)[5], 94.5 kJ/mol ($\Delta_f H°$, gas)[5]		
Heat of combustion	−28.37 kJ/g (exptl.)[3], −1,305.2 ± 0.59 kJ/mol ($\Delta_c H°$, liq., static bomb calorimetry)[5], −1,305.2 kJ/mol ($\Delta_c H°$, liq., calorimetry)[5]		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]			
T_{ex} [K]			
$p_{C\text{-}J}$ [kbar]			

VoD [m s^{-1}]			
V_0 [L kg^{-1}]			
Thermal stability	Stable under the extremes of heat and cold expected in long-term storage[2], stable up to its atmospheric boiling point in absence of oxygen[2]		
Vapor pressure [atm. @ °C]	6.3 kPa @ 25 °C[1], 49.63 mm Hg @ 25 °C[2]		
Viscosity [centistokes]	0.893[2]		
Compatibility	Catalysts such as rust, Cu or copper alloys can cause dec.[2]		
Heat of vaporization [cal/mol]	9,648 @ 25 °C[2]		
Specific heat [cal/mol K]	32.35 @ 25 °C[2], 134.93 J/mol K (constant pressure heat capacity of liq. @ 298.15 K)[5]		
ΔH_{dec} [kJ/mol]	−4.340 kJ/g (max. heat of dec., calcd., CHEETAH)[3], −22.01 kJ/g (heat of dec., calcd., CHEETAH)[3]		

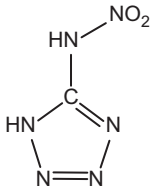
	MMH[4]
Chemical formula	CH_6N_2
Molecular weight [g mol^{-1}]	46.07
Crystal system	Monoclinic
Space group	$P2_1/c$
a [Å]	10.043(10)
b [Å]	3.925(5)
c [Å]	7.670(8)
α [°]	90
β [°]	107.28(10)
γ [°]	90
V [$Å^3$]	288.7(6)
Z	4
ρ_{calc} [g cm^{-3}]	1.06
T [K]	179

[1] U. Schaller, T. Keicher, J. Hürttlen, V. Weiser, H. Krause, S. Schlechtriem, *Investigation of Gelled Ionic Liquid as Hypergolic Fuels*, ICT **2011**, Karlsruhe, Germany, pp. 87-1–87-7.
[2] P. J. von Doehren, *Propellant Handbook*, AFRPL-TR-66-4, Air Force Rocket Propulsion Laboratory Research and Technology Division, United States Air Force, California, USA, January **1966**.
[3] S. G. Pakdehi, S. Rezaei, H. Motamedoshariati, M. H. Keshavarz, *J. Loss Prevention in the Process Industries*, **2014**, *29*, 277–282.
[4] M. Foulon, N. Lebrun, M. Muller, A. Amazzal, M. T. Cohen-Adad, *Acta Cryst.*, **1994**, *B50*, 472–479.
[5] P. J. Lindstrom,W. G. Mallard, *NIST Chemistry WebBook*, NIST Standard Reference Database, National Institute of Standards and Technology, Gaithersburg, USA, webbook.nist.gov.

N

5-Nitraminotetrazole

Name [German, acronym]: Nitraminotetrazole [5-nitraminotetrazol]
Main (potential) use: gas generant
Structural formula:



	5-Nitraminotetrazole		
Formula	$CH_2N_6O_2$		
Molecular mass [g mol^{-1}]	130.07		
Appearance at room temperature (RT)			
IS [J]			
FS [N]			
ESD [J]			
N [%]	64.61		
$\Omega(CO_2)$ [%]	−12.30		
$T_{m.p.}$ [°C]			
$T_{dec.}$ [°C]			
ρ [g cm^{-3}]	1.828 (X-ray @ 295 K)[2]		
Heat of formation			
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]			
T_{ex} [K]			
$p_{C\text{-}J}$ [kbar]			

https://doi.org/10.1515/9783110672565-013

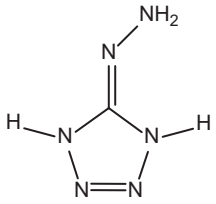
VoD [m s^{-1}]			
V_0 [L kg^{-1}]			
Burn rate [mm/s]	Values from Russian FLAME database[1]: 10.0 mm/s @ 3.5 atm pressure[1], 11.0 mm/s @ 10 atm[1], 50.0 mm/s @ 40 atm[1], 200.0 mm/s @ 110 atm[1]		
Solubility [g/mL]			

	5-Nitraminotetrazole[2]
Chemical formula	$CH_2N_6O_2$
Molecular weight [g mol^{-1}]	130.02
Crystal system	Monoclinic
Space group	$P2_1/c$
a [Å]	9.40
b [Å]	5.56
c [Å]	9.36
α [°]	90
β [°]	105.00
γ [°]	90
V [$Å^3$]	472.522
Z	4
ρ_{calc} [g cm^{-3}]	1.828
T [K]	295

[1] R. L. Simmons, C. M. Walsh, *Designing Advanced Gun Propellants with Improved Energy-Release*, ICT **2001**, Karlsruhe, Germany, pp. 43-1–43-11.
[2] J. H. Bryden, *Acta Cryst.*, **1953**, *6*, 669–670.

5-Nitriminotetrazole

Name [German, acronym]: 5-Nitrimino-1,4*H*-tetrazole, [5-nitriminotetrazol]
Main (potential) use:
Structural formula:



	5-Nitriminotetrazole		
Formula	$CH_2N_6O_2$		
Molecular mass [g mol^{-1}]	130.09		
Appearance at RT	Colorless crystals[1]		
IS [J]	1.5 (75–125 µm grain size, BAM)[1]		
FS [N]	8 (75–125 µm grain size, BAM)[1]		
ESD [J]	0.19[1]		
N [%]	64.61		
$\Omega(CO_2)$ [%]	−12.3		
$T_{m.p.}$ [°C]			
$T_{dec.}$ [°C]	122 (exotherm, DSC @ 5 °C/min)[1]		
ρ [g cm^{-3}]	1.867 (X-ray @ 100 K)[1]		
Heat of formation	322 kJ/mol ($\Delta_f H°$)[1], 264 kJ/mol ($\Delta_f H°$)[1]		
Heat of combustion	−1,700 cal/g[1]		
	Calcd. (EXPLO5 5.02)	Lit. values	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]	5,746[1]		
T_{ex} [K]	4,563[1]		
$p_{C\text{-}J}$ [kbar]	394[1]		
VoD [m s^{-1}]	9,450 (@ 1.867 g cm^{-3})[1]		
V_0 [L kg^{-1}]	800[1]		

ΔH_{dec} [J/g]	2,638 (exptl.)[1]
pK_a	2.5 and 6.1 (dibasic acid)[1]
Long-term stability tests	Stable long-term, no exotherm in 48 h @ 80 °C (RADEX V5 oven)[1]

	5-Nitriminotetrazole[1]
Chemical formula	$CH_2N_6O_2$
Molecular weight [g mol^{-1}]	130.09
Crystal system	Monoclinic
Space group	$P2_1/c$ (no. 14)
a [Å]	9.4010(3)
b [Å]	5.4918(1)
c [Å]	9.3150(3)
α [°]	90
β [°]	105.762(3)
γ [°]	90
V [Å^3]	462.84(2)
Z	4
ρ_{calc} [g cm^{-3}]	1.867
T [K]	100
	Colorless crystals from H_2O/HNO_3

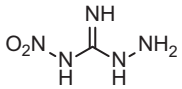
[1] J. Stierstorfer, *Advanced Energetic Materials Based on 5-Aminotetrazole – Synthesis, Characterization and Scale-Up*, PhD Thesis, LMU München, Munich, **2009**.

Nitroaminoguanidine

Name [German, acronym]: *N´*-Nitrohydrazinecarboximidamide, *N´*-nitro-*N*-aminoguanidine, 1-amino-3-nitro-guanidine, aminonitroguanidine [NAGu, ANQ]

Main (potential) use: Oxidizer

Structural formula:



	NAGu	
Formula	$CH_5N_5O_2$	
Molecular mass [g mol^{-1}]	119.08	
Appearance at RT		
IS [J]	20 (BAM)[3], 3 Nm[4], 22 cm (2 kg mass)[5]	
FS [N]	144 (BAM)[3], 240[4]	
ESD [J]	0.15 (@ 100–500 µm grain size, ESD 2010 EN)[3]	
N [%]	58.8	
$\Omega(CO_2)$ [%]	–33.6	
$T_{m.p.}$ [°C]	184 (dec.)[3, 5]	
$T_{dec.}$ [°C]	190[1], 184 (DSC @ 5 °C/min, covered Al container with hole in lid)[3], 184 (melts with dec.)[5], 190 (explosion)[5]	
ρ [g cm^{-3}]	1.71 (@ 298 K), 1.722 (crystal @ 173 K)[3]	
Heat of formation	161.7 kJ/mol ($\Delta_f H°$ (g), calcd., CBS-4M)[3], + 185.5 kJ/kg (enthalpy of form.)[4], 76.9 kJ/mol ($\Delta_f H°$ (s), calcd.)[3], 5.30 kcal/mol (Q_f^V)[5], –43.4 kcal/kg[6], 22.1 kJ/mol (enthalpy of form., exptl.)[7], –16.6 kJ/mol (enthalpy of form., calcd., emp.)[7], 4.1 kJ/mol (enthalpy of form., calcd., S-D method)[7]	
Heat of combustion	270.14 kcal/mol (Q_c^V)[5], 2,250 kcal/kg (@ C^V)[6]	
	Calcd. (EXPLO5 5.04)	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]	4,915 (@ 1.722 g cm^{-3}) [3]	3,746 [H_2O (l)][4] 3,418 [H_2O (g)][4]

T_{ex} [K]	3,310 (@ 1.722 g cm^{-3}) [3]	
$p_{C\text{-}J}$ [kbar]	307 (@ 1.722 g cm^{-3}) [3]	
VoD [m s^{-1}]	8,729 (@ 1.722 g cm^{-3})[3]	
V_0 [L kg^{-1}]	878 (@ 1.722 g cm^{-3})[3]	

Sand test [g]	39.8 g sand crushed (cf. 43.0 g for TNT)[3]
5 s explosion T [°C]	190[3]
100 °C heat test [% mass loss]	0.12% mass loss in first 48 h[3], 0.15% in second 48 h[3], no explosion in 100 h[3]
Vacuum stability test [cm^3/h]	>11 cc gas produced in 16 h @ 120 °C[3]
Solubility [g/mL]	Poor solubility in water, can be recryst. from hot water[3], recryst. from 40% HF in H_2O[3], soluble in DMSO[3]

	NAGu[2]
Chemical formula	$CH_5N_5O_2$
Molecular weight [g mol^{-1}]	119.09
Crystal system	Tetragonal[2]
Space group	
a [Å]	17.063
b [Å]	17.063
c [Å]	5.155
α [°]	90
β [°]	90
γ [°]	90
V [Å^3]	
Z	
ρ_{calc} [g cm^{-3}]	
T [K]	

[1] R. A. Henry, R. C. Makosky, G. B. L. Smith, *J. Am. Chem. Soc.*, **1951**, *73*, 474–474.
[2] S. R. Naidu, N. M. Bhide, K. V. Prabhakaran, E. M. Kurian *J. Therm. Anal.*, **1995**, *44*, 1449–1462.
[3] N. Fischer, T. M. Klapötke, J. Stierstorfer, *Z. Naturforsch.*, **2012**, *67b*, 573–578.
[4] R. Meyer, J. Köhler, A. Homburg, *Explosives*, 7th edn., Wiley-VCH, Weinheim, **2016**, p. 226.

[5] B. T. Fedoroff, H. A. Aaronson, E. F. Reese, O. E. Sheffield, G. D. Clift, *Encyclopedia of Explosives and Related Items*, *vol. 1*, US Army Research and Development Command, TACOM, Picatinny Arsenal, USA, **1960**.

[6] Y. Y. Orlova, *The Chemistry and Technology of High Explosives, Part III*, translated by the Technical Documents Liaison Office, Wright Patterson Air Force Base, Ohio, Technical AD261783, Armed Services Technical Information Agency, Virginia, USA, 23rd June **1961**.

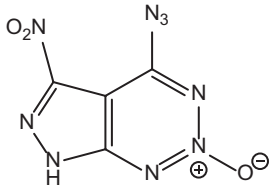
[7] B. Nazari, M. H. Keshavarz, M. Hamadanian, S. Mosavi, A. R. Ghaedsharafi, H. R. Pouretedal, *Fluid Phase Equilibria,* **2016**, *408*, 248–258.

6-Nitro-7-azido-pyrazol[3,4-d][1,2,3]triazine-2-oxide

Name [German, acronym]: 6-Nitro-7-azido-pyrazol[3,4-d][1,2,3]triazine-2-oxide, [ICM-103]

Main (potential) use: Possible future environmentally friendly primary explosive[1]

Structural formula:



	ICM-103		
Formula	$C_4HN_9O_3$		
Molecular mass [g mol^{-1}]	223.11		
Appearance at RT	Light yellow solid (crude)[1]		
IS [J]	4 (0.02 g sample, powder predried @ 60 °C for 2 h, sample pressed with screw press @ 39.2 MPa pressure, BAM)[1]		
FS [N]	60 (20–30 mg sample, sample pre-treated @ 50 °C for 4 h, ceramic test plate, BAM)[1]		
ESD [J]	130 (20–30 mg sample, pretreated @ 50 °C for 4 h)[1]		
N [%]	56.50		
$\Omega(CO_2)$ [%]	−39.44		
$T_{dec.}$ [°C]	160.3 (onset) 180.5 (exo peak max) (DSC @ 10 °C/min)[1]		
ρ [g cm^{-3}]	1.86 (gas pycnometry @ 25 °C)[1], 0.37 (bulk ρ @ 25 °C)[1]		
Heat of formation	744.75 kJ/mol (calcd., Byrd and Rice method)[1], 739.40 kJ/mol (measured, heat of comb. expts.)[1]		
Heat of combustion	$\Delta_c U_m^\theta = -11{,}066$ J/g (−2,468.81 kJ/mol) (exptl. constant vol. combustion energies)[1]		
	Calcd. (EXPLO5 6.02)	Lit. values	Exptl.

$-\Delta_{ex}U°$ [kJ kg^{-1}]	−5,964.86 (@ 1.86 g cm^{-3}, heat of form. = 744.75 kJ/mol)[1]		
T_{ex} [K]	4,347 (@ 1.86 g cm^{-3}, heat of form. = 744.75 kJ/mol)[1]		
$p_{C\text{-}J}$ [kbar]	35.1 GPa (@ 1.86 g cm^{-3}, heat of form. = 744.75 kJ/mol)[1]		
VoD [m s^{-1}]	9,111 (@ 1.86 g cm^{-3}, heat of form. = 744.75 kJ/mol)[1]		
V_0 [L kg^{-1}]	709 (@ 1.86 g cm^{-3}, heat of form. = 744.75 kJ/mol)[1]		
Initiation efficiency	Minimum primary charge = 60 mg, actual charge = 90–100 mg ICM-103 can detonate PET and RDX to bore through lead plate (5 mm thick lead plate, ICM-103 filled in no. 8 blasting cap, pressed by 32 MPa static pressure, fired by standard pyrotechnical igniter)[1]		
Thermal stability	Long-term stability test: <5 mg per ~ 2 g sample weight loss after 48 h @ 75 °C under atmospheric pressure, and no changes in appearance or particle morphology visible using optical microscopy[1]		
Solubility [g/mL]	Insoluble in water[1], 0.08 g/100 mL H_2O @ 25 °C[1]		
Hygroscopicity	Nonhygroscopic[1], 0.18 wt.% after 24 h in humidity chamber[1]		
Photosensitivity	Insensitive to light[1], maintains high purity even after long exposure to sunlight[1]		
Compatibility	Insensitive to moisture[1]		
Flame test	Flame sensitivity H_{50} ≥60 cm (H_{50} reflects the reliability of ignition)[1]		
Flowability	θ = 28.76°, satisfactory flowability[1]		
Dead pressed/ pressure durability	>100 MPa (below this value ICM-103 is dead pressed)[1]		

	ICM•H_2O[1]
Chemical formula	$C_4H_3N_9O_4$
Molecular weight [g mol^{-1}]	241.15
Crystal system	Monoclinic
Space group	$P2_1/c$ (no. 14)

a [Å]	9.931(5)
b [Å]	5.210(3)
c [Å]	19.767(7)
α [°]	90
β [°]	116.419(19)
γ [°]	90
V [Å^3]	915.9(8)
Z	4
ρ_{calc} [g cm^{-3}]	1.749
T [K]	173
	Crystals of hydrate from slow evaporation of soln. in methanol

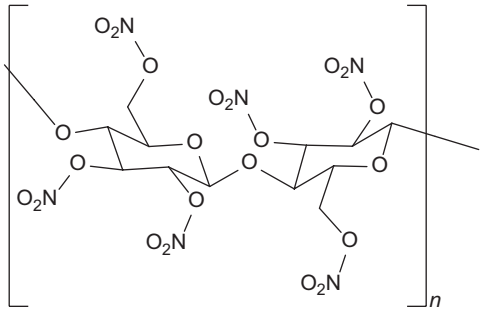
[1] M. Deng, Y. Feng, W. Zhang, X. Qi, Q. Zhang, *Nature Comm.*, **2019**, *1*0, Article nr. 1339.

Nitrocellulose

Name [German, acronym]: Nitrocellulose*, cellulose nitrate [Nitrozellulose, Cellulosenitrat, Zellulosenitrat, Schießbaumwolle, Bitzwatte, NC]

Main (potential) use: Blasting explosive, smokeless powder, component for propellants, single base in small arms, grenade, artillery[24], component of double-base powders in small arms, mortars and artillery rockets[24], used as a component of multibase powders as cool burning gun propellant[24]

Structural formula:



* Complete nitration forms cellulose trinitrate with 14.14% N[18]

Collodion (pyroxylin) is a NC with ~ 8–12% N and is soluble in Et_2O/EtOH[18]; NC which contains 8–12.3% N[28], pyroxylin is the only NC which is not used in explosives.[4]
Pyrocellulose contains 12.6% N [18]; NC with a N content of 12.60 ± 0.10%.[28]
Guncotton is NC containing ≥13% N [18]; the grade of NC that contains the highest % N using mixed nitric and sulfuric acids as the nitrating agents, N content = 13.35–13.45%.[28]
CP_1 is NC which contains ~ 13% N.[18]
CP_2 is NC which contains ~ 12% N.[18]
Nitrocellulose (cellulose nitrate) is a mixture of nitrates obtained by nitrating cellulose.[28]
High nitrogen cellulose is NC which contains 13.75–14.14% N.[28]
Blended NC is a mixture of 60–65% guncotton (with 13.4% N content) and 35–40% pyrocellulose (with 12.6% N content)[28]; two grades of NC are commonly used: (i) 13.15 ± 0.05% N content and (ii) 13.25 ± 0.05% N content.[28]

<table>
<tr><td></td><td>NC (some data refer to structural unit)</td></tr>
<tr><td></td><td></td></tr>
<tr><td>Formula</td><td>$C_{12}H_{14}N_6O_{22}$ (if complete nitration occurs)</td></tr>
<tr><td>Molecular mass [g mol^{-1}]</td><td>Nitrocellulose (12.60): 544.79
Nitrocellulose (13.45): 572.68
Nitrocellulose(14.14): 594.3</td></tr>
<tr><td>Appearance at RT</td><td>NC powders: hard, horn-like, manufactured in various forms such as strips, flakes, pellets varying in color from translucent pale yellow to opaque brown or black[24]. Pyroxylin: light yellow, matted filaments[28], white when pure but usually appears amber, brown or black colored[4], manufactured as flakes, strips, sheets, pellets or perforated cylindrical grains[4], odorless and tasteless solid polymer[33], white with rubular structure fibers which are hard and glossy[33]</td></tr>
<tr><td>IS [J]</td><td>Nitrocellulose (12.60% N): 8 cm (2 kg mass, 20 mg sample, B.M.)[4, 5, 6], 3 in (2 kg mass, 5 mg sample, P.A.)[4, 5, 6]
Nitrocellulose (13.45% N): 9 cm (2 kg mass, 20 mg sample, B.M.)[4, 5, 6], 3 in (2 kg mass, 5 mg sample, P. A.)[4, 5, 6]
Nitrocellulose (13.45% N, gun cotton): 3 in (2 kg mass, P.A.)[7], 9 cm (B.M.)[7]
Nitrocellulose (14% N): 3 in (2 kg mass, 5 mg sample, P.A.)[7], 8 cm (B.M.)[7]
Nitrocellulose (14.14% N): 1.57 (8 cm, 2 kg mass, 20 mg sample, B.M.)[6], 1.50 (3 in, 2 kg mass, 5 mg sample, P.A.)[6]
8 cm (for all types of NC)[28]</td></tr>
<tr><td>FS [N]</td><td>353</td></tr>
<tr><td>ESD [J]</td><td>Highest ESD energy @ 5,030 V for zero ignition probability (NC, 13.4% N)[9]:
<table>
<tr><td colspan="2">Highest E (J) for zero ignition probability</td><td colspan="2">Type of ignition</td></tr>
<tr><td>Unconfined</td><td>Confined</td><td>Unconfined</td><td>Confined</td></tr>
<tr><td>0.061</td><td>3.1</td><td>Deflag.</td><td>Deflag.</td></tr>
</table></td></tr>
<tr><td>N [%]</td><td>Nitrocellulose (12.60): 12.60
Nitrocellulose (13.45): 13.45
Nitrocellulose(14.14): 14.14</td></tr>
<tr><td>$\Omega(CO_2)$ [%]</td><td>Nitrocellulose (12.60): −35
Nitrocellulose (13.45): −29
Nitrocellulose(14.14): −24</td></tr>
<tr><td>$T_{m.p.}$ [°C]</td><td>Nitrocellulose (14.14): decomposition[6]
Nitrocellulose (13.45): decomposition[6]
Nitrocellulose (12.60): decomposition[6]
NC powders (all types) do not melt[24], 206 (MWt. = 10^5–10^6)[27], >135 (with dec., pyroxylin with 12% N content)[28], >135 (with dec. for guncotton)[28], does not melt[33]</td></tr>
</table>

<table>
<tr><td>$T_{dec.}$ [°C]</td><td>206.57 (DSC @ 10 °C/min, NC 12.52% N)[22]</td></tr>
<tr><td>ρ [g cm^{-3}]</td><td>1.67 (@ 298 K), 1.550[1], 1.65–1.70 (NC 14.14% N)[6], 1.66 (NC 14.14% N)[26], 1.7092 (NC 12.56% N)[22], 1.66 (NC 13.15% N)[26], 1.66 (NC 12.6% N)[26], 1.653 (TMD for pyroxylin with 12% N content)[28], 1.656 (TMD for guncotton)[28], 1.659 (TMD for high nitrogen cellulose)[28], 1.65–1.66 (with increasing N content)[33]</td></tr>
<tr><td>Heat of formation</td><td>–669.8 kJ/mol[2]
Nitrocellulose (14.14% N): 617 cal/g[6], ΔH_f = –653 kJ/mol[26]
Nitrocellulose (13.45% N): 561 cal/g[6], ΔH_f = –678 kJ/mol[26]
Nitrocellulose (13.15% N): ΔH_f = –688 kJ/mol[26]
Nitrocellulose (12.60% N): 617 cal/g[6], ΔH_f = –708 kJ/mol[26]

–2,581.5 kJ/kg[1], –216 kcal/mol (pyroxylin with 12% N content)[28], –200 kcal/mol (guncotton with 13.35% N content)[28], –191 kcal/mol (high nitrogen cellulose with 14.14% N content)[28]

Values for the enthalpy of formation from literature sources, cited in ref.[19]:

<table>
<tr><th>% N</th><th>Condition of preparation of samples</th><th>$-\Delta H°_f$ (NC) kcal/kg</th></tr>
<tr><td>10.24</td><td>Dried @ 110 °C in vacuum, 3 h, sealed in polyethylene packages</td><td>778.1</td></tr>
<tr><td>11.56</td><td>Dried @ 110 °C in vacuum, 3 h, sealed in polyethylene packages</td><td>696.3</td></tr>
<tr><td>12.28</td><td>Not dried
dried on air
dried @ 110 °C in vacuum, 1 h, pressed as tablets</td><td>656.0</td></tr>
<tr><td>13.41</td><td>Dried on air
dried @ 110 °C in vacuum, 3 h, sealed in polyethylene packages</td><td>586.4</td></tr>
<tr><td>13.49</td><td>Dried @ 110 °C in vacuum, 1 h, maintained day on air
dried @ 110 °C in vacuum, 1 h, sealed in polyethylene packages</td><td>576.9</td></tr>
<tr><td>13.65</td><td>Dried @ 110 °C in vacuum, 3 h, sealed in polyethylene packages</td><td>562.6</td></tr>
</table>
</td></tr>
</table>

Values for the heat of formation from literature sources, cited in[11]:

% N content	Heat of formation (kcal/kg)	Comments	% N content	Heat of formation (kcal/kg)	Comments
7.66	958.9	Calcd., *Tomioka*	13.53	594	Calcd., *Lenze et al.*
10.14	804.1	Calcd., *Tomioka*	13.58	568.7	Calcd., *Tomioka*
11.06	742.3	Calcd., *Tomioka*	13.92	513	Calcd., *Lenze et al.*
12.45	645.2	Calcd., *Tomioka*	14.12	504	Calcd., *Lenze et al.*
12.88	616.5	Calcd., *Tomioka*			
10	759.6	No. of nitro groups in relation to C_6 = 1.71; MWt. of C_6 unit = 238.8	13	562.3	No. of nitro groups in relation to C_6 = 2.58; MWt. of C_6 unit = 278.3
11	694.3	No. of nitro groups in relation to C_6 = 1.97; MWt. of C_6 unit = 250.6	14	496.6	No. of nitro groups in relation to C_6 = 2.94; MWt. of C_6 unit = 294.6
12	628.1	No. of nitro groups in relation to C_6 = 2.26; MWt. of C_6 unit = 263.8			

–2,390 kJ/kg (ΔH_f, NC = 13.4% N; ICT thermochemical database)[20],
–2,598 kJ/kg (ΔH_f, NC = 12.6% N; ICT thermochemical database)[20],
–2,859 kJ/kg (ΔH_f, NC = 11.6% N; ICT thermochemical database)[20]

See additional values at end of section[33]
†See figure at end of this section[14]

Heat of combustion [kJ mol^{-1}]

2,409 cal/g (NC 12.6% N)[6], 2,313 cal/g (NC 13.45% N)[6], 2,228 cal/g (NC 14.14% N)[6], 651,800 cal/mol (Q_c^v, NC 12.6% N)[7], 2,409 kcal/kg (NC 12.6% N)[8], 649,000 cal/mol (Q_c^v, NC 13.45% N)[7], 2,313 kcal/kg (NC 13.45% N)[8], 2,303 kcal/kg (Q_c^v, NC 13.45% N)[8], 647,000 cal/mol (Q_c^v, NC 14.14% N)[7], 2,228 kcal/kg (NC 14.14% N)[8], 2,322 cal/g (Q_c^P, NC 14%)[7], 2,242 cal/g (Q_c^v, NC 14%)[7]

values for the heat of combustion from literature sources, cited in[11]:

% N content	Heat of combustion (kcal/kg)	Comments	% N content	Heat of combustion (kcal/kg)	Comments
7.66	3,071	Calcd., *Tomioka*	13.53	2,236	Calcd., *Lenze et al.*
10.14	2,717	Calcd., *Tomioka*	13.58	2,286	Calcd., *Tomioka*
11.06	2,612	Calcd., *Tomioka*	13.92	2,239	Calcd., *Lenze et al.*
12.45	2,434	Calcd., *Tomioka*	14.12	2,208	Calcd., *Lenze et al.*
12.88	2,390	Calcd., *Tomioka*			

Heat of combustion decreases with increasing N content[33], see additional values at end of the section.[33]

	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
	NC 13.25%		
$-\Delta_{ex}U°$ [kJ kg^{-1}]	4,642	1,025 kcal/kg[3] 4,500 kJ/kg (NC 13.4% N, calcd. thermochem.)[13] 3,385 kJ/kg (NC 11.2% N, calcd. thermochem.)[13] >1,025 kcal/kg (guncotton, 13.1% N, *Kast*)[16]	Nitrocellulose (12.6% N): 855 cal/g[6] Nitrocellulose (13.45% N): 965 cal/g[6, 8] Nitrocellulose (14.14% N): 1,058 cal/g[6] Nitrocellulose (14.14% N): Q_e (calcd./exptl. not specified) = 2,228 cal/g[8]

		973 cal/g (12.62% N, calcd. based on exptl. values) [H_2O (l)][11] 865 cal/g (12.62% N, calcd. based on exptl. values) [H_2O (g)][11] 1,025 cal/g (13.0% N, calcd. based on exptl. values) [H_2O (l)][11] 925 cal/g (13.0% N, calcd. based on exptl. values) [H_2O (g)][11] 1,046 cal/g (13.15% N, calcd. based on exptl. values) [H_2O (l)][11] 946 cal/g (13.15% N, calcd. based on exptl. values) [H_2O (g)][11] 1,055 cal/g (13.2% N, calcd. based on exptl. values) [H_2O (l)][11] 955 cal/g (13.2% N, calcd. based on exptl. values) [H_2O (g)][11] 1,096 cal/g (13.45% N, calcd. based on exptl. values) [H_2O (l)][11] 955 cal/g (13.45% N, calcd. based on exptl. values) [H_2O (g)][11] 1,056 kcal/kg (est. based on exptl. values)[11] 4,409 J/g (NC 13.4% N, calcd., ICT code)[20] 3,983 J/g (NC 12.6% N, calcd., ICT code)[20]	1.16 kcal/g (Pyroxylin, 12% N) [H_2O (l)][28] 1.02 kcal/g (Pyroxylin, 12% N) [H_2O (g)][28] 1.16 kcal/g (guncotton, 13.35% N) [H_2O (l)][28] 1.02 kcal/g (guncotton, 13.35% N) [H_2O (g)][28] 1.95 cal/mol (high nitrogen cellulose, 14.14% N) [H_2O (l)][28] 1.81 kcal/mol (high nitrogen cellulose, 14.14% N) [H_2O (g)][28]

		3,480 J/g (NC 11.6% N, calcd., ICT code)[20] 4,288.6 (NC 13.1% N)[33] 3,661 (NC 13.1% N, 16% H_2O)[33]	
T_{ex} [K]	3,325	3,100[3] 3,447 (NC 13.4% N, calcd. thermochem.)[13] 2,586 (NC 11.2% N, calcd. thermochem.)[13] 3,100 °C (guncotton, 13.1% N, *Kast*)[16] 2,840 °C (12.62% N, calcd. based on exptl. values)[11] 3,025 °C (13.0% N, calcd. based on exptl. values)[11] 3,095 °C (13.15% N, calcd. based on exptl. values)[11] 3,130 °C (13.2% N, calcd. based on exptl. values)[11] 3,245 °C (13.45% N, calcd. based on exptl. values)[11] 3,388 (NC 13.4% N, calcd., ICT code)[20] 3,085 (NC 12.6% N, calcd., ICT code)[20] 2,683 (NC 11.6% N, calcd., ICT code)[20] 3,100 °C (NC 13.1% N)[33]	

		2,260 (NC 13.1% N, 16% H_2O)[33] Increases with increasing N content[33]	
$p_{C\text{-}J}$ [kbar]	23.4	121.8 MPa (NC 13.4% N, calcd., ICT code)[20] 115.7 MPa (NC 12.6% N, calcd., ICT code)[20] 106.3 MPa (NC 11.6% N, calcd., ICT code)[20]	
VoD [m s^{-1}]	7,459	6,300 (@ 1.3 g cm^{-3})[3] 6,300 (@ 1.3 g cm^{-3}, NC 13.1% N)[33] 6,800 (@ 1.3 g cm^{-3}, NC 13.1% N, 16% H_2O)[33]	Nitrocellulose (13.45% N): 7,300 (@ 1.20 g cm^{-3})[4, 6, 12] 6,300 (@ 1.30 g cm^{-3}, guncotton)[11] 6,800 (guncotton containing 16% H_2O)[11]
V_0 [L kg^{-1}]	709	765 (@ 0 °C)[3] 765 (guncotton, 13.1% N, Kast)[16] 900 cm^3/g (12.62% N, calcd. based on exptl. values) [H_2O (l)][11] 880 cm^3/g (13.0% N, calcd. based on exptl. values) [H_2O (l)][11] 874 cm^3/g (13.15% N, calcd. based on exptl. values) [H_2O (l)][11] 868 cm^3/g (13.2% N, calcd. based on exptl. values) [H_2O (l)][11] 857 cm^3/g (13.45% N, calcd. based on exptl. values) [H_2O (l)][11]	871 Nitrocellulose (12.6% N): 919[6] Nitrocellulose (13.45% N): 883[6] Nitrocellulose (14.14% N): 853[6]

		720 (NC 13.1% N, 16% H_2O)[33] Decreases with increasing N content[33]	

Nitrocellulose 12.6% N:
Q_E^V = 941 cal/g[7], V_0 = 0.04041 mol/g[7], Q_E (calcd./exptl. not specified) = 855 kcal/kg[7], heat of formation = 617 kcal/kg[7], ρ = 1.655 g cm^{-3}[7]

Nitrocellulose 13.45% N:
Q_E = 1,061 cal/g[7], V_0 = 0.03854 mol/g[7], ρ = 1.657 g cm^{-3}[7]

Nitrocellulose 13.45% N (guncotton):
VoD = 7,300 (@ 1.20 g cm^{-3})[7], V_0 = 712 mL/g [H_2O (l)][7], V_0 = 883 mL/g [H_2O (g)][7], Q_E^V = 1,063 cal/g [H_2O (l)][7], Q_E^V = 982 cal/g [H_2O (g)][7], Q_f^P = 551 cal/g[7]

Nitrocellulose 14% N:
V_0 = 688 mL/g [H_2O (l)][7], V_0 = 854 mL/g [H_2O (g)][7], V_0 (calcd.) = 838 mL/g [H_2O (g)][7], Q_E^V = 1,137 cal/g [H_2O (l)][7], Q_E^V = 1,059 cal/g [H_2O (g)][7], Q_E^V (calcd.) = 1,051 cal/g [H_2O (g)][7], Q_f^P = 516 cal/g[7]

Nitrocellulose 14.14% N:
Heat of detonation (calcd./exptl. not specified) = 1,486 kcal/kg[8], Q_E = 1,160 cal/g[7], V_0 = 0.03704 mol/g[7], ρ = 1.659 g cm^{-3}[7]

Data from[33]:

	N content of NC (%)				
	12.62	13.0	13.15	13.2	13.45
Explosion heat (J/g) (liq. H_2O)	4,071	4,288.6	4,376.5	4,414.1	4,585.7
Explosion heat (J/g) (vapor H_2O)	3,619.2	3,870.2	3,958.1	3,995.7	4,029.2
Specific volume, V_0 (mL/g) (liq. H_2O)	900	880	874	868	857
Detonation T (°C)	2,840	3,025	2,095	3,130	3,245

The combustion heat and heat of formation of NC with different nitrogen contents[33]:

N content of NC (%)	Combustion heat (J/g)	Heat of formation (J/g)
7.66	12,849.07	4,012
10.14	11,367.93	3,364.36
11.06	10,928.61	3,105.79
12.45	10,183.86	2,699.52
12.88	9,999.76	2,579.44
13.53	9,773.83	2,485.30
13.58	9,489.32	2,379.44
13.92	9,367.98	2,146.4
14.12	9,238.28	2,108.74

Detonation velocity of low-density nitrocellulose/nitroglycerine charges; PMMA = polymethyl methacrylate with 6 mm wall thickness, * average velocity over entire length of charge[25]:

System	NC/NG ratio	Confinement		Foam density (g/cc)	Explosive density (g/cc)	Detonation velocity (mm/μs)
		Type	I.D., cm			
Foamed NC/NG	50/50	PMMA	2.54	0.255	0.191	Unstable
	50/50	Steel	5.08	0.134	0.121	0.66
	50/50	Steel	5.08	0.173	0.118	0.42
	50/50	Steel	5.08	0.103	0.083	0.62
	50/50	Steel	5.08	0.103	0.074	0.72
	50/50	Steel	5.08	0.130	0.057	0.70*
NC/NG mixture	97/3	PMMA	2.54	–	0.191	2.6
	87/13	PMMA	2.54	–	0.191	2.6
	77/23	PMMA	2.54	–	0.191	2.7
	60/40	PMMA	2.54	–	0.225	2.74
Fibrous NC	100/0	Aluminum	7.52	–	0.174	2.51
Expanded NC	100/0	PMMA	2.54	–	0.252	1.88
	100/0	PMMA	2.54	–	0.141	2.31
	100/0	PMMA	2.54	–	0.104	2.07

Calculated detonation pressure of low-density nitrocellulose/NG charges; PMMA = polymethyl methacrylate with 6 mm wall thickness, gage pressure was calcd. using equations[25]:

System	Explosive ρ (g/cc)	Foam ρ (g/cc)	Minimum gage resistance (ohms)	Gage pressure (kbars)	PMMA pressure (kbars)	Detonation pressure (kbars)
Expanded NC	0.252	–	264	8.3	8.6	4.8
	0.141	–	324	4.6	5.1	2.8
	0.104	–	399	1.8	2.2	1.2
97/3 NC/NG	0.191	–	94.5	14.4	18.2	–
87/13 NC/NG	0.191	–	81.7	17.3	20.9	–
77/23 NC/NG	0.191	–	87.8	15.8	19.5	–
60/40 NC/NG	0.225	–	74.0	19.5	23.4	–

Trauzl test [cm^3, % TNT]	325–420 cc (NC 13% N)[10], 136–147% TNT (NC 13.2–13.4% N)[7, 28], 373 cm^3 (NC, 13.4% N)[31], 375 (NC 13.1% N)[33], 280 cm^3 (NC 13.1% N, 16% H_2O)[33]
Sand test [g]	45.0 g (200 g bomb, NC 12.6% N)[4, 6], 49.0 g (200 g bomb, NC 13.45% N)[4, 6], 52.3 g (200 g bomb, NC 14.14% N)[6], comparable with that of TNT[28], 49 g sand crushed (NC 13.45% N, cf. 48 g for TNT)[7], 52 g sand crushed (cf. 48 g for TNT)[7], 109–120% TNT (NC ~ 14% N)[7], 105% TNT (NC 13.2–13.4% N)[7], 94–98% TNT (NC 12.6% N)[7]
Ballistic mortar test	125% TNT (NC 13.45% N)[4, 6, 7], 118% TNT (NC 13.2–13.4% N)[7], 118% TNT (guncotton)[28]
LSGT [cm]	H = hydraulic press, regular test, all charges conditioned and fired at 25 °C[30]:

Material	Density		50% point		Particle size (µm)	Comments
	g/cc	% TMD	Cards	kbar		
NC	1.45 H	91.8	197	(20)	314	Contains 12.6% N

Initiating efficiency	NC 12.6% N: 0.10 g LA minimum detonating charge[6], NC 13.45% N: 0.10 g LA minimum detonating charge[6], NC 14.14% N: 0.10 g LA minimum detonating charge[6], can be detonated by initiating compounds or boosters[24]

<table>
<tr><td>5 s explosion T [°C]
5 s ignition T [°C]</td><td>230 (NC 13.34% N)[7], 170 (pyrocellulose)[28], 200 (blended NC)[28], 230 (guncotton)[28]
170 (dec., NC 12.6% N)[6, 8], 222 (NC 13.3% N)[8], 230 (NC 13.45% N)[6, 8]</td></tr>
<tr><td>Explosion T [°C]</td><td>Explosion T @ various times of exposure (25 mg sample, ignition or deflagration) T(°C)/exposure time (s)[11]:
NC 13.4% N: 292/0.38, 264/1.30, 234/5.80, 198/41.4, 174/120, 170/no action[11]
NC 12.6% N: 350/1.48, 312/5.50, 286/16.6, 267/50.3, 260/no action[11]</td></tr>
<tr><td>Ignition T [°C]</td><td>187[17]

T (°C) and time to explosion (s), 25 mg sample, 13.4% N[23]:

<table><tr><td>T (°C)</td><td>Time (s)</td><td>T (°C)</td><td>Time (s)</td></tr><tr><td>358</td><td>0.074</td><td>210</td><td>21.5</td></tr><tr><td>331</td><td>0.100</td><td>198</td><td>41.1</td></tr><tr><td>292</td><td>0.383</td><td>185</td><td>201</td></tr><tr><td>264</td><td>1.30</td><td>180</td><td>440</td></tr><tr><td>242</td><td>3.99</td><td>174</td><td>1,200</td></tr><tr><td>234</td><td>5.80</td><td>170</td><td>No explosion</td></tr><tr><td>225</td><td>10.2</td><td></td><td></td></tr></table>
T (°C) and time to explosion (s), 25 mg sample, 12.6% N[23]:

<table><tr><td>T (°C)</td><td>Time (s)</td><td>T (°C)</td><td>Time (s)</td></tr><tr><td>325</td><td>0.143</td><td>210</td><td>21.5</td></tr><tr><td>287</td><td>0.442</td><td>192</td><td>76.5</td></tr><tr><td>246</td><td>2.87</td><td>188</td><td>102</td></tr><tr><td>243</td><td>4.20</td><td>180</td><td>458</td></tr><tr><td>227</td><td>8.17</td><td>170</td><td>No explosion</td></tr><tr><td>218</td><td>13.7</td><td></td><td></td></tr></table></td></tr>
<tr><td>100 °C heat test [% mass loss]</td><td>0.3% mass loss in first 48 h (NC 13.45% N)[6, 7], 0.0% mass loss in second 48 h (NC 13.45% N)[6, 7], no explosion in 100 h (NC 14.35% N)[6], 11 + cc in 24 h (NC 14% N)[7]</td></tr>
<tr><td>65.5 °C KI test</td><td>35 min (minimum) (pyrocellulose)[28], 35 min (minimum) (blended NC)[28]</td></tr>
<tr><td>134 °C heat test</td><td>30 min (minimum) (pyrocellulose)[28], 30 min (minimum) (bonded NC)[28]</td></tr>
</table>

<table>
<tr>
<td>Thermal stability</td>
<td>
Effect of heating on NC (from 1 g of guncotton)[15]:
<table>
<tr><th>Heating T (°C)</th><th>Heating time (h)</th><th>Vol. of (g) produced (cm^3)</th><th>Weight loss (%)</th><th>N loss (%)</th></tr>
<tr><td>125</td><td>150</td><td>162</td><td>49.7</td><td>64</td></tr>
<tr><td>135</td><td>150</td><td>236</td><td>61.8</td><td>83</td></tr>
<tr><td>140</td><td>40</td><td>310</td><td>66.5</td><td>91</td></tr>
<tr><td>150</td><td>20</td><td>325</td><td>70.2</td><td>98</td></tr>
</table>
Rapid dec. >100 °C[28], very slow dec. even @ RT[28] and rate of dec. increases 3.71 × per 10 °C temperature increase[28], can be stored <100 °C without dec. for long term[33]

Storage lifetime predictions, NC used; viscosity average molecular weight = 511 ± 7%, nitrogen content = 12.53 ± 0.02%, degree of substitution = 2.42, crystallinity index = 22.9%[34]:
<table>
<tr><th></th><th colspan="3">S1_NC</th></tr>
<tr><th></th><th>Years</th><th>Months</th><th>Days</th></tr>
<tr><td>Unaged</td><td>10</td><td>10</td><td>29</td></tr>
<tr><td>Aged 40 days</td><td>2</td><td>1</td><td>9</td></tr>
<tr><td>Aged 80 days</td><td>–</td><td>1</td><td>25</td></tr>
<tr><td>Aged 120 days</td><td>–</td><td>1</td><td>0</td></tr>
</table>
</td>
</tr>
<tr>
<td>Vacuum stability test [cm^3/h]</td>
<td>
NC 12.6% N: 0.17 cc/40 h @ 90 °C[6], 1.0 cc/40 h @ 100 °C[6], 11 + cc/16 h @ 120 °C[6]
NC 13.45% N: 0.42 cc/40 h @ 90 °C[6], 1.5 cc/40 h @ 100 °C[6], 11 + cc/40 h @ 120 °C[6]
NC 14.14% N: 1.46 cc/40 h @ 90 °C[6], 11 + cc/14 h @ 100 °C[6], 11 + cc/16 h @ 120 °C[6]

1.5 cc gas evolved from 5 g sample (NC 13.45% N)[7], 1.46 cc gas evolved @ 90 °C[7], 2.84 mL/g (@ 100 °C, 48 h, NC = 12.56% N)[22]
</td>
</tr>
</table>

Heating CP_1 in vacuum @ 75 °C (all gas volumes have been reduced to 0 °C and 760 mm Hg)[18]:

Duration of heating (days)	Total vol. (cm^3)	cm^3 gas per g per day
1st period, 5 days	2.25	0.0128
2nd period, 5 days	17.29	0.0088
3rd period, 5 days	18.55	0.00927
4th period, 5 days	18.34	0.0080
5th period, 5 days	18.19	0.0079
6th period, 5 days	18.3	0.0084

After 309 days heating @ 75 °C, oven was reduced to 40 °C (vacuum) and same sample is heated for 221 days. Total gas evolved during this time = 0.697 cc (i.e. 0.0001154 cc per gram per day). The sample was then heated in vacuum @ 100 °C[18]:

Duration of heating (hours)	Total vol. (cm^3)	cm^3 gas per g per day
1st period @ 100 °C, 30 h	29.09	0.662
2nd period @ 100 °C, $8^1/_2$ h	8.57	0.689
3rd period @ 100 °C, 9 h	8.09	0.614

6 cm^3/48 h @ 120 °C (NC with 12% N content)[28]

NC used; viscosity average molecular weight = 511 ± 7%, nitrogen content = 12.53 ± 0.02%, degree of substitution = 2.42, crystallinity index = 22.9%[34]:

Designation	VST			
	V_{gases} released (mL/g)			
	UN	A40 days	A80 days	A120 days
NC T = 353.15 K	1.52	4.84	5.19	6.83
T = 363.15 K	1.60	6.85	7.98	9.88
T = 373.15 K	1.85	15.97	17.15	18.09
T = 383.15 K	4.06	18.51	23.24	25.07

NC used; viscosity average molecular weight = 514.783 ± 7%, nitrogen content = 12.56 ± 0.03%, degree of substitution = 2.44, crystallinity index = 23.7%[36]: Vol. released gases = 1.62 ± 0.02 mL/g

<table>
<tr><td>Vapor pressure [atm @ °C]</td><td>0.0 mm Hg @ 60 °C (NC 13.45% N)[7], 0.0 mm Hg @ 60 °C (NC 14% N)[7]</td></tr>
<tr><td>Volatility [mg/cm^2/h]</td><td>0.0 @ 60 °C (NC 12.6% N)[6], 0.0 @ 60 °C (NC 13.45% N)[6], 0.0 @ 60 °C (NC 14.14% N)[6]</td></tr>
<tr><td>Burn rate [mm/s]</td><td>7.0 @ 100 atm pressure[21], 50.0 @ 100 atm[21], 100.0 @ 2,000 atm[21], NC powders burn rapidly and have detonated under confinement or when burned in deep piles, burn rate varies considerably with composition, initial T and pressure under which burning occurs[24], pyroxylin is highly flammable[28], 0.3 (@ 1 atm, SMATCH/FTIR spectroscopy, 13% N NC)[32], 0.4 (@ 1 atm, strand burner, 13% N NC)[32]</td></tr>
<tr><td>Solubility [g/mL]</td><td>Data from[6]
<table>
<tr><td></td><td>12.6% N</td><td>13.45% N</td><td>14.0% N</td></tr>
<tr><td colspan="4">Solubility in H_2O (g/100 g) at</td></tr>
<tr><td>25 °C</td><td>Insoluble</td><td>Insoluble</td><td>Insoluble</td></tr>
<tr><td>60 °c</td><td>Insoluble</td><td>Insoluble</td><td>Insoluble</td></tr>
<tr><td colspan="4">Solubility (g/100 g) @ 25 °C in</td></tr>
<tr><td>Ether</td><td>Insoluble</td><td>Insoluble</td><td>Insoluble</td></tr>
<tr><td>Alcohol</td><td>Very slightly soluble</td><td>Practically insoluble</td><td>insoluble</td></tr>
<tr><td>2:1-Ether:alcohol</td><td>Soluble</td><td>Slightly soluble (6–11%)</td><td>Practically insoluble (1 +%)</td></tr>
<tr><td>Acetone</td><td>Soluble</td><td>Soluble</td><td>Soluble</td></tr>
</table>
Soluble in acetone, acetic esters[15], collodion is soluble in Et_2O-EtOH[18, 28], guncotton is insoluble in ether-alcohol, soluble in acetone and ethyl acetate[18], CP_1 is insoluble in ether-alcohol[18], CP_2 is soluble in ether-alcohol[18], NC (with N content >11%) is rel. poorly soluble in alcohol[11], acetone does not dissolve NC with N <10%[11], NC with N <10% dissolves in dilute aqueous NaOH[11], NC with N ≥10% is completely soluble in ethyl acetate[11], NC with 11.8% N shows 99.3% solubility in ether-alcohol[11], NC with 12% N shows 99.5% solubility in ether-alcohol[11], NC with 12% N shows 99.7% solubility in ether-alcohol[11], NC with 11.9% N shows 99.3% solubility in ether-alcohol[11], NC with 11.8% N shows 98.5% solubility in ether-alcohol[11], most NC powders are soluble in Et_2O/EtOH mixture or acetone[24], insoluble in H_2O @ 25 °C (Mwt. = 10^5–10^6)[27],

Pyroxylin is soluble in acetone or glacial acetic acid[28]

Pyrocellulose is insoluble in Et_2O and water[28], 99% dissolves in 2:1 soln. of Et_2O/EtOH[28], 21% dissolves in ethyl nitroacetate[28], 11% dissolves in EtOH[28], pyrocellulose is soluble in acetone, ethyl acetate, methyl acetate, propylene oxide, nitromethane and nitroethane[28]</td></tr>
</table>

Guncotton is insoluble in water and Et_2O[28], very slightly soluble in EtOH[28], 4–10% soluble in Et_2O/EtOH (2:1) soln.[28], soluble in acetone, ethyl acetate and other common organic solvents[28]

High-nitrogen cellulose is insoluble in water, Et_2O, *n*-propyl alcohol, and ^{i}PrOH[28], 0.6% soluble in EtOH, 1% soluble in MeOH, 1.4% soluble in Et_2O/EtOH (2:1) soln., 20% soluble in methyl acetate, 42% soluble in nitromethane, 86% soluble in 1-nitropropane and 100% soluble in acetone, ether acetate, propylene oxide and amyl acetate[28]

Blended NC is 37% soluble in Et_2O/EtOH (2:1) soln.[28]

Classes of compounds which can dissolve NC[11]:

Class of compound	Examples	Class of compound	Examples
Alcohols	MeOH, EtOH, PrOH	Organic acid esters	Carbonates e.g,. ethylcarbonate, formats, acetates e.g., ethyl acetate, oxalates, maleates, carbamates
Aldehydes	Acetalaldehyde, benzaldehyde, furfural	*N*-substituted carbonamides	Acetanilide, urea derivatives
Ketones	Acetone, methyl ethyl ketone, propione, acetophenone, cyclohexanone, camphor	Aliphatic nitro	Nitroparaffins e.g., NM, nitroethane
Ethers	$MeONO_2$, Et_2O, Pr_2O Bu_2O, ethers in mixtures with alcohols	Aromatic nitro	Nitrobenzene, nitrotoluene, dinitrobenzene, dinitrotoluene, TNT, nitroanisoles, dinitroanisoles
Inorganic acid esters	Nitrates e.g.. $MeONO_2$, nitrogylcol, NG, silicate e.g., ethyl silicate, phosphates *e.g.,* triphenylphosphate	Heterocycles	Pyridine

<table>
<tr><td></td><td>Best ether-alcohol mixtures for NC with different % N contents[11]: % N content = 11.80, optimum vol. ether:alcohol ratio = 50:50[11], % N content = 12.20, optimum vol. ether:alcohol ratio = 53:47[11], % N content = 12.55, optimum vol. ether:alcohol ratio = 70:30[11]

NC (12.2 or 12.6% N) is soluble, that is, miscible in all proportions with Et_2O/EtOH (2:1 v/v)[29], NC (13.4% N) poorly soluble in Et_2O/EtOH (2:1 v/v)[29]</td></tr>
<tr><td>Viscosity [s]</td><td>180 (% N content = 11.8)[11], 160 (% N content = 12)[11], 138 (% N content = 12)[11], 102 (% N content = 11.9)[11], 93 (% N content = 11.8)[11], 447 (% N content = 9.09)[11], 1,800 (% N content = 10.41)[11], 16,200 (% N content = 12.48)[11], 18,600 (% N content = 13.02)[11], 322,500 (% N content = 13.5)[11]

Influence of exposure to light on the viscosity of NC[11]:

<table>
<tr><th>Time of exposure to light (h)</th><th>Viscosity of NC (s)</th><th>Time of exposure to light (h)</th><th>Viscosity of NC (s)</th></tr>
<tr><td>–</td><td>335</td><td>480</td><td>270</td></tr>
<tr><td>24</td><td>320</td><td>900</td><td>240</td></tr>
<tr><td>48</td><td>305</td><td></td><td></td></tr>
</table></td></tr>
<tr><td>Hygroscopicity</td><td>3% @ 30 °C, 90% RH (NC 12.6% N)[6], ~ 2% @ 30 °C, 90% RH (NC 13.45% N)[6], ~ 1% @ 30 °C, 90% RH (NC 14.14% N)[6], pyrocellulose: 3% @ 30 °C with 90% RH[28], blended NC (13.15% N): 2.5% @ 30 °C with 90% RH[28], guncotton (13.45% N): 2% @ 30 °C with 90% RH[28], high nitrogen cellulose (14% N): 1% @ 30 °C with 90% RH[28], NC is somewhat hygroscopic but hygroscopicity decreases with increasing nitrogen content[4]

The lower the % N content of NC, the more hygroscopic it is[15]

Tendency of NC powder to uptake moisture (on exposure to an atmosphere almost saturated with water)[18]:

<table>
<tr><td>Period of exposure (h)</td><td>0</td><td>24</td><td>48</td><td>72</td><td>96</td></tr>
<tr><td>External moisture (%)</td><td>1.02</td><td>1.15</td><td>1.40</td><td>1.47</td><td>1.57</td></tr>
</table>
Effect of alcohol on colloided pyrocellulose powder: colloidal pyrocellulose absorbs alcohol from an atmosphere saturated with alcohol vapor[18]; values for sample of colloidal pyrocellulose powder before and after exposure to atmospheres saturated with H_2O or alcohol[18]:</td></tr>
</table>

Method of determining external moisture and residual solvent	Exposure to H_2O residual solvent		Exposure to alcohol residual solvent	
	Before	After	Before	After
1 h @ 100 °C in open oven	3.12	2.82	2.41	4.57
6 h @ 100 °C in open oven	2.81	2.36	2.22	3.92
6 h @ 55 °C in vacuum	2.91	2.54	2.27	4.10
55 °C to constant weight in open oven	3.00	2.72	2.58	4.25
Over sulfuric acid to constant weight	2.95	2.39	2.32	4.10

Most NC powders are hygroscopic and moisture accelerates dec.[24]

Hygroscopicity of NC for NC used in propellants (saturated atmosphere @ 25 °C), data from[29]:

N in NC (%)	H_2O (%)
13.40	1.19
13.15	1.57
12.60	2.36
12.2ß	2.91

Photosensitivity

Influence of exposure to light on the viscosity of NC[11]:

Time of exposure to light (h)	Viscosity of NC (s)	Time of exposure to light (h)	Viscosity of NC (s)
–	335	480	270
24	320	900	240
48	305		

Pyroxylin is dec. by light[28]

Compatibility

Dec. by addition of NC to an excess of 10% aqueous NaOH solution @ 70 °C[6], effect of alcohol of colloided pyrocellulose powder: colloidal pyrocellulose absorbs alcohol from an atmosphere saturated with alcohol vapor[18], most NC powders are hygroscopic and moisture accelerates dec.[24], pyroxylin with 11.13% N hydrolyzes @ 1.71% of available nitrogen in 240 h in boiling water[28], pyrocellulose with 12.6% N hydrolyzes @ 1.22% of available nitrogen in 240 h in boiling water[28], guncotton with 13.44% N hydrolyzes @ 1.03% of available nitrogen in 240 h in boiling water[28], highly compatible with MENA, DPA but degree of incompatibility with ANA (NC used synthesized from Alfa grass fibers)[35]

Decomposition of NC, thermal stability values under different conditions from[28]:

Decomposition medium	% available nitric acid liberated per hour at	
	50 °C	97.5 °C
Heat	0.0000045	0.0028
Water	0.0000111	0.0051
0.06% nitric acid soln.	0.0000325	
0.035% nitric acid soln.	–	0.0088
0.035% sodium carbonate soln.	0.0006870	0.1358
95% ethanol	0.0000290	

NC used; viscosity average molecular weight = 511 ± 7%, nitrogen content = 12.53 ± 0.02%, degree of substitution = 2.42, crystallinity index = 22.9%[34]:

Designation		VST				Bergmann and Junk (T = 405.15 K)			
		V_{gases} released (mL/g)				V_{NOx} released (mL/g)			
		UN	A40 days	A80 days	A120 days	UN	A40 days	A80 days	A120 days
NC + MENA	T = 353.15 K	1.16	1.38	1.50	1.61	0.63	1.01	1.20	1.48
	T = 363.15 K	1.25	1.45	1.62	1.73				
	T = 373.15 K	1.36	1.68	2.02	2.42				
	T = 383.15 K	2.76	5.44	6.69	7.04				
NC + DPA	T = 353.15 K	0.91	1.00	1.28	1.57	0.62	0.97	1.19	1.47
	T = 363.15 K	0.99	1.15	1.32	1.64				
	T = 373.15 K	1.18	1.38	1.90	2.31				
	T = 383.15 K	2.10	4.85	5.94	6.38				
NC + (MENA + DPA)	T = 353.15 K	1.02	1.11	1.32	1.61	0.59	0.86	1.07	1.38
	T = 363.15 K	1.07	1.21	1.46	1.69				
	T = 373.15 K	1.21	1.45	1.96	2.29				
	T = 383.15 K	2.06	4.72	6.00	6.35				

Storage lifetime predictions, NC used; viscosity average molecular weight = 511 ± 7%, nitrogen content = 12.53 ± 0.02%, degree of substitution = 2.42, crystallinity index = 22.9%[34]:

	NC			NC + MENA			NC + DPA			NC + (MENA + DPA)		
	Years	Months	Days	Years	Months	Days	Years	Months	Days	Years	Months	Days
Unaged	10	10	29	24	4	11	26	7	23	27	11	5
A_40 days	2	1	9	18	2	18	20	11	9	22	8	25
A_80 days	–	1	35	4	8	1	8	4	10	12	2	13
A_120 days	–	1	0	4	0	12	4	11	23	6	11	15

NC used; viscosity average molecular weight = 514.783 ± 7%, nitrogen content = 12.56 ± 0.03%, degree of substitution = 2.44, crystallinity index = 23.7%, Bergmann and Junk and VST obtained results[36]:

Designation	Bergmann and Junk		VST
	V_{NaOH} (mL/g)	V_{NO} released (mL/g)	V released gases (mL/g)
NC	4.79 ± 0.09	1.07 ± 0.02	1.62 ± 0.02
NC + MENA	2.72 ± 0.04	0.61 ± 0.01	1.10 ± 0.02
NC + DPA	3.20 ± 0.08	0.72 ± 0.02	0.90 ± 0.02
NC + (MENA + DPA)	2.23 ± 0.04	0.50 ± 0.01	1.04 ± 0.02

Bergmann-Junk [mL/g]

1.08 (vol. of NO gas released, 0.5 g sample @ 132 °C for 5 h, NC 12.56% N)[22]

NC used; viscosity average molecular weight = 511 ± 7%, nitrogen content = 12.53 ± 0.02%, degree of substitution = 2.42, crystallinity index = 22.9%[34]:

Bergmann & Junk (T = 405.15 K)			
V_{NOx} released (mL/g)			
UN	A40 days	A80 days	A120 days
1.18	2.16	2.98	3.72

NC used; viscosity average molecular weight = 514.783 ± 7%, nitrogen content = 12.56 ± 0.03%, degree of substitution = 2.44, crystallinity index = 23.7%[36]:

Designation	Bergmann and Junk	
	V_{NaOH} (mL/g)	V_{NO} released (mL/g)
NC	4.79 ± 0.09	1.07 ± 0.02

Specific heat [cal/g/°C]	Pyrocellulose = 0.3478 @ 25 °C[28], guncotton (13.4% N) = 0.3408 @ 25 °C[28], high nitrogen cellulose (14.14% N) = 0.3362[28]
Rifle bullet impact test	Detonation in 100% of trials[28]
LLNL test	1.0–1.2 cm^3/0.25 g sample (NC)[28]

	NC trinitrocellulose[15]	**NC intermediate structure for % N of 12.3–13.2 (*Trommel*)[15]**	**NC trinitrate structure (*Trommel*)[15]**
Chemical formula			
Molecular weight [g mol^{-1}]			
Crystal system	Orthorhombic		
Space group			
a [Å]	12.40	13.81	12.94
b [Å]	25.4	10.45	25.66
c [Å]	9.0	7.92	892
α [°]	90		
β [°]	90	90	
γ [°]	90		
V [$Å^3$]			
Z			
ρ_{calc} [g cm^{-3}]			
T [K]			

Crystal cell dimensions along the (101) axis for various NCs (Miles)[15]:

Compound	% N	*d*/Å along (101) (eq.) axis
Cellulose nitrated to:	11.14	6.67
	12.77	6.85
	13.57	7.25
NC 13.75%, denitrates to	11.52	7.10
NC 13.75%, denitrates to	10.42	7.05

Fig. 13 from[14]

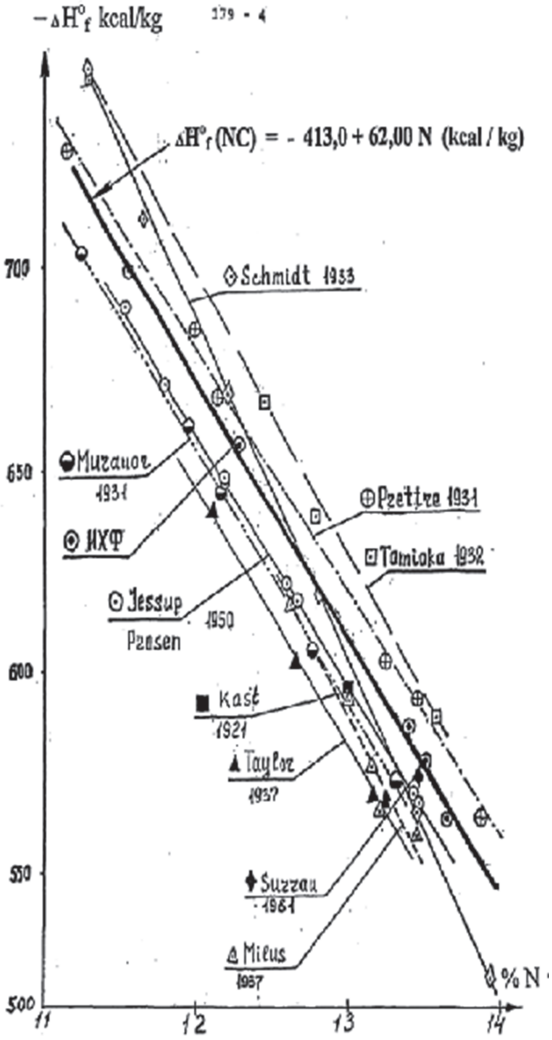


Fig. 13: The dependence of the enthalpy of formation of NC on percentage nitrogen.[14]

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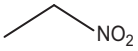
Nitroethane

Name [German, acronym]: Nitroethane, nitrous acid ethyl ester, nitrous ether [nitroethan]

Main (potential) use: Secondary (high) explosive, melt cast

Structural formula:



	Nitroethane	
Formula	$C_2H_5NO_2$	
Molecular mass [g mol^{-1}]	75.07	
Appearance at RT	Colorless or yellowish clear, flammable, highly volatile liquid with characteristic burning sweet taste[6]	
N [%]	18.66	
Ω(CO_2) [%]	−95.9	
$T_{m.p.}$ [°C]	114	
$T_{b.p.}$ [°C]	114.0[5], 114[7]	
ρ [g cm^{-3}]	1.05[1], 1.0352 (@ 293 K)[2], 1.053[3], 1.041[4], sp. gr. = 1.047 (@ 15 °C)[5], $d^{15}{}_{15} = 0.90$[6]	
Heat of formation	−1,917.4 kJ/kg (enthalpy of form.)[3], −1,849.3 kJ/kg[4], −24.5 kcal/mol (ΔH_f(g)°, calcd., ccCA-P)[8], −26.3 kcal/mol (ΔH_f(g)°, calcd., ccCA-S3)[8], −25.4 kcal/mol (ΔH_f(g)°, calcd., ccCA-PS3)[8], −25.5 kcal/mol (ΔH_f(g)°, calcd., G3)[8], −23.8 kcal/mol (ΔH_f(g)°, calcd., G3(MP2))[8], −24.4 ± 1.0 kcal/mol (ΔH_f(g)°, exptl.)[8]	
	Calcd. (EXPLO5 6.04)	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]	3,930	1,686 [H_2O (l)][3] 1,608 [H_2O (g)][3]
T_{ex} [K]	2,535	
$p_{C\text{-}J}$ [kbar]	93.1	
VoD [m s^{-1}]	5,798 (@ 1.045 g cm^{-3}, $\Delta_f H = -142$ kJ mol^{-1})	
V_0 [L kg^{-1}]	955	

Thermal stability	Gradual dec. on storage whereby dec. is increased by air, light and moisture[6]
Solubility [g/mL]	Readily soluble in benzene, toluene, xylene, EtOH and acetone[5], slightly soluble in water (with dec.)[6], miscible with EtOH, Et_2O[6]
Photosensitivity	Gradual dec. on storage is increased by exposure to light, store with protection from light[6]
Refractive index	1.3901 (@ 24 °C)[5]

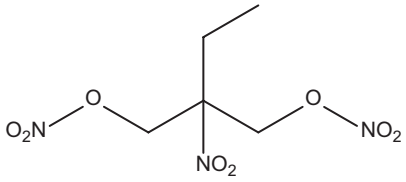
[1] Hazardous Substances Data Bank, obtained from the National Library of Medicine (US).
[2] G. A. Shvekhgeimer, *Zh. Org. Khim.*, **1966**, *10*, 1852–1856.
[3] R. Meyer, J. Köhler, A. Homburg, *Explosives*, 7th edn., Wiley-VCH, Weinheim, **2016**, p. 229.
[4] https://engineering.purdue.edu/~propulsi/propulsion/comb/propellants.html
[5] Y. Y. Orlova, *The Chemistry and Technology of High Explosives, Part II*, translated by the Technical Documents Liaison Office, Wright Patterson Air Force Base, Ohio, Technical AD261783, Armed Services Technical Information Agency, Virginia, USA, 23rd June **1961**.
[6] *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**.
[7] J. Liu, *Nitrate Esters Chemistry and Technology*, Springer, **2019**.
[8] K. R. Jorgensen, G. A. Oyedepo, A. K. Wilson, *J. Hazard. Mater.*, **2011**, *186*, 583–589.

Nitroethylpropanediol dinitrate

Name [German, acronym]: 2-Nitro-2-ethyl-1,3-propanediol dinitrate, 1,1-dimethylol-1-nitropropane dinitrate, 2-ethyl-2-nitro-1,3-propanediol dinitrate [Nitroethylpropandiolnitrat]

Main (potential) use: Secondary (high) explosive, melt cast

Structural formula:



	Nitroethylpropanediol dinitrate	
Formula	$C_5H_9N_3O_8$	
Molecular mass [g mol^{-1}]	239.14	
Appearance at RT	Liquid[7]	
IS [J]	Slightly less sensitive than NG[5], lower than that of PA[7]	
N [%]	17.57	
Ω(CO_2) [%]	−43.5	
$T_{m.p.}$ [°C]	335.3 ± 37.0[1]	
ρ [g cm^{-3}]	1.474 ± 0.06 (@ 293 K)[1], 1.44[3], 1.443 (@ 20 °C)[4], sp. gr. = 1.443 (@ 20/20°)[5]	
Heat of formation	−367.2 ± 4.2 kJ/mol ($\Delta_f H°_{solid}$)[2], −82.7 kcal/kg (@ C^V)[5], −88.5 kcal/kg (@ C^P)[5], −367.4 kJ/mol (enthalpy of form., exptl.)[8], −364.6 kJ/mol (enthalpy of form., calcd., emp.)[8], −384.9 kJ/mol (enthalpy of form., calcd., S-D method)[8]	
Heat of combustion	$\Delta_c H°_{solid}$ = −2,886.5 ± 4.2 kJ/mol[2], −693.5 kcal/kg (@ C^V)[5], −691.5 kcal/kg (@ C^P)[5]	
	Calcd. (EXPLO5 6.03)	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]	5,012	4,340 [H_2O (l)][3]
T_{ex} [K]	3,416	
$p_{C\text{-}J}$ [kbar]	20.1 GPa	

VoD [m s^{-1}]	7,205 (@ TMD)	
V_0 [L kg^{-1}]	818	1,032[3]

Trauzl test [cm^3, % TNT]	125% PA[7]
Ballistic mortar test	92% of blasting gelatin[4, 6]
Thermal stability	Withstands 82.2 °C for 5 min[4, 6]
Volatility	10 g sample left in crystallizer @ 40 °C for several days showed an average loss of 1.08 mg per sq decimeter of surface[5]
Viscosity [cP]	49 (@ 20 °C)[5]

[1] Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994–2017 ACD/Labs).

[2] P. J. Linstrom, W. G. Mallard, *NIST Chemistry WebBook*, NIST Standard Reference Database Number 69, July **2001**, National Institute of Standards and Technology, Gaithersburg, MD, 2014, 20899, www.webbook.nist.gov.

[3] R. Meyer, J. Köhler, A. Homburg, *Explosives*, 7th edn., Wiley-VCH, Weinheim, **2016**, pp. 229–230.

[4] B. T. Fedoroff, O. E. Sheffield, *Encyclopedia of Explosives and Related Items*, *vol. 5*, US Army Research and Development Command, TACOM, Picatinny Arsenal, USA, **1972**.

[5] B. T. Fedoroff, O. E. Sheffield, *Encyclopedia of Explosives and Related Items*, *vol. 6*, US Army Research and Development Command, TACOM, Picatinny Arsenal, USA, **1974**.

[6] S. M. Kaye, *Encyclopedia of Explosives and Related Items*, *vol. 8*, US Army Research and Development Command, TACOM, Picatinny Arsenal, USA, **1978**.

[7] J. Liu, *Nitrate Esters Chemistry and Technology*, Springer, **2019**.

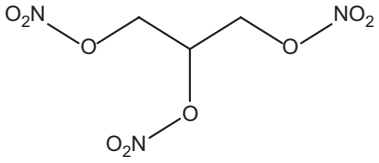
[8] B. Nazari, M. H. Keshavarz, M. Hamadanian, S. Mosavi, A. R. Ghaedsharafi, H. R. Pouretedal, *Fluid Phase Equilibria,* **2016**, *408*, 248–258.

Nitroglycerine

Name [German, acronym]: 1,2,3-Propanetriol trinitrate, glycerol trinitrate [nitroglycerin, nitroglyzerin, Sprengol, NG, PTTN]

Main (potential) use: Gelatinous industrial explosives, component of powders, gun propellants and smokeless solid rocket propellants, main component of dynamites[32], ingredient in mining explosives[32], component of smokeless double-base propellants[32], can be used directly as high-explosive[50], blasting of oil wells[50], manufacture of dynamite and propellants[50], propellant compositions[7], dynamites[7], blasting explosive (in combination with non-explosive materials)[7]

Structural formula:



	NG
Formula	$C_3H_5N_3O_9$
Molecular mass [g mol^{-1}]	227.09
Appearance at RT	Colorless oily transparent liquid (pure)[7, 32, 55, 59], commercial is usually yellowish or pale brown liquid[7, 32, 55], stable form = dipyramidal rhombic crystals[33], labile form = glassy-appearing triclinic crystals[33], colorless–yellow–pale brown liquid, color depends on purity[50], clear, colorless, odorless, oily liquid[20], technical product is usually yellowish or yellow-brown oily liquid[59], sweetish and burning taste and sweetish odor[59], liquid[65], colorless, oily liquid; industrial NG usually light yellow or light brown (depends on the purity of raw materials and production method)[69]

IS [J]

0.2 Nm[13, 43], 15 cm (2.94 J, 2 kg mass, 20 mg sample, B.M.)[7, 8, 9], 0.55 (1 cm, 1 lb mass, P.A.)[8, 9], 2 cm (2 kg mass, Kast apparatus), 44 cm (2 kg mass)[15], 4 cm (2 kg mass, B.M.)[15], 15 cm (2 kg mass, B.M.)[16], 1 in (1 lb mass, 20 mg sample, P.A.)[17], 8–10 cm (samples absorbed on filter paper, 2 kg mass, Kast apparatus)[7], 70 cm = minimum fall (50 g mass, B.M.)[17], 10–12 cm (2 kg mass, *Stettbacher*)[33], NG @ 90° requires only 50% of the drop[33], frozen NG requires three times as much drop as NG @ RT[33], 8–10 cm (2 kg mass, drop absorbed on filter paper)[33], 70 cm (500 g mass, *Rinkenbach* using small drop machine)[33], 1 cm (Julius-Peters)[35], 20 cm (Bruceton method, type 12 tool, 2.5 kg mass, 40 mg sample, 5/0 sandpaper, 25 trials)[37], H_{50} = 15 cm[39], <1.0 Nm (1 kg hammer, 10 cm, lower testing value not possible on ICT apparatus, strong bang)[41], <1.0 Nm (1 kg hammer, 10 cm, lower testing value not possible on ICT apparatus, strong bang, liq., $^{6}/_{6}$ positive tests, @ 20 °C, 51% air humidity)[44], H_{50} = 20 cm (2.5 kg mass, type 12 tool)[46], 3.5 cm (2 kg mass, ~ 25 mg sample)[47], 20–30 cm (0.5 kg, NG powder)[53], force of ≥100 g/cm with 5 cm diameter weight (P.A.)[20], frozen NG is much less sensitive than liquid NG and sensitivity increases as temperature increases[20], most sensitive is NG crystals in contact with NG liquid[20], readily detonated if iron strikes iron or if porcelain strikes porcelain[59], 4 cm (2 kg mass), heated NG more sensitive[59], $H_{50\%}$ = 4 cm (2.5 kg mass)[67]

Olin apparatus, liquid NG[21]:

Dropping mass (kg)	Drop height (cm)	No. of trials	No. of initiations
1	1.0	20	0
1.5	1.0	10	5
1	2.0	10	4
1	3.0	10	9

Olin apparatus, solid NG, carried out @ 5–10 °C[21]:

Dropping mass (kg)	Drop height (cm)	No. of trials	No. of initiations
2.0	32	20	0
3.0	32	18	1
3.0	48	10	2

Olin apparatus, solid/liquid mixtures of NG, carried out @ 5–10 °C[21]:

Dropping mass (kg)	Drop height (cm)	No. of trials	No. of initiations
2.0	32	10	0
2.0	48	10	1

NG/acetone mixtures, B.M.[20]:

Composition, %		Impact test (cm)
100	0	16
90	10	23
80	20	41
75	25	60
73	27	64
70	30	100 +

Data from[69]

Phase	Impact force (kg m/cm^2)	Explosion rate (%)
Liquid	0.08	10
	0.11	50
	0.40	100
Stable crystallite	0.51	10
	0.65	50
	0.82	100
Unstable crystallite	0.63	10
	0.78	50
	0.93	100

FS [N]

Explodes with steel shoe (friction pendulum test)[9], 360, >353[13], sensitive on rubbing in a porcelain mortar with rough surface[32], torpedo friction = >150 cm (1 kg @ 80 °C, 0.5 m/s)[34], friction wheel = >50 kg (1 kg @ 80 °C, 0.5 m/s)[34], minimum hot spot temperature for ignition by friction = 450–480 °C[34], >36 kg (Julius-Peters)[35], 112 (tiny flames)[41], 112 (tiny flames, $^1/_6$ positive tests, @ 20 °C, 51% air humidity)[44], 18 lb @ 3 ft/s (ABL)[4], >150 cm (NG powder, torpedo friction, 1 kg @ 80 °C)[53], >50 kg (NG powder, friction wheel, 0.5 ms^{-1})[53], more sensitive to friction when frozen[59], wood mallet on stone = 100%[63], wood mallet on soft wood = 0%[63], wood mallet on hard wood = 0%[63], NG prepared with deionized water is less sensitive and can withstand the friction on the surface of a mortar[69]

<table>
<tr><td>ESD [J]</td><td>>12.5 (unconfined)[9]

Highest ESD energy @ 5,000 V for zero ignition probability[16]:

<table>
<tr><td></td><td colspan="2">Highest E (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>NG @ 25 °C > 12.5</td><td>0.90</td><td>None</td><td>Deton.</td><td></td></tr>
<tr><td>NG @ 60 °C</td><td>–</td><td>0.056</td><td>None</td><td>Deton.</td></tr>
</table>

NG (liquid) or saturated on filter paper: no ignition or explosion from a 13 kV spark from an 8 µF condenser[17], @ 50–60 °C NG liquid or NG liquid saturated in filter paper does not explode or ignite from a 13 kV spark from an 8 micro farad capacitor[20]</td></tr>
<tr><td>N [%]</td><td>18.50</td></tr>
<tr><td>Ω(CO_2) [%]</td><td>+3.5</td></tr>
<tr><td>$T_{m.p.}$ [°C]</td><td>13.2 (stable modification)[7, 9, 16, 35, 50, 55, 62], 2.2 (unstable (labile) modification)[7, 9, 16, 35, 50, 55, 62], lower mpt. = labile form[32], higher mpt. = stable form[32], 10.2–13.8 (visual mpt., purified)[18], 9.6–13.2 (visual mpt., sample as received)[18], 10.9 (onset endotherm, DSC @ 10 °C/min)[18], 13.2–13.5 (stable form)[33], 1.9–2.2 (labile form)[33], 13.2[39, 49], 13[43, 63], 13.5[57], 13.5 (rhombic crystals, stable form)[20], 2.8 (glassy triclinic crystals, labile form)[20], 13[67], 189.5 (onset), 192.1 (peak max), 193.9 (end T) (DSC @ 10.0 K/min, pinhole cover)[48]

Freezing points from different sources, values in °C[32, 69]:

<table>
<tr><td>Form</td><td>Nauckhoff</td><td>Kast</td><td>Hibbert</td><td>Hackel</td></tr>
<tr><td>Labile</td><td>–</td><td>2.1–2.2</td><td>1.9</td><td>1.9</td></tr>
<tr><td>Stable</td><td>12.4</td><td>13.2</td><td>13.0</td><td>13.0</td></tr>
</table>

Freezing point = 13.2 (stable form, rhombic crystals)[20], freezing point = 2.1 (labile form, glassy triclinic crystals)[20], freezing point (labile form) = 2.1 °C[59], mpt. (labile) = 2.8 °C[59], freezing point (stable form) = 13.2 °C[59, 65], mpt. (stable) = 13.5 °C[59], 13.2 (solidification point, stable modification, orthorhombic)[65], 2.2 (solidification point, less stable modification, triclinic)[65], 2.1 (crystallization T of melt for α form) and 2.8 (mpt., α form)[66], 13.2 (crystallization T of melt for β form) and 13.5 (mpt., β-form)[66]</td></tr>
</table>

<table>
<tr><td></td><td>Solidification rates into the stable form @ different T[69]:

<table><tr><td>T (°C)</td><td>Rate (mm/min)</td></tr><tr><td>5</td><td>0.145</td></tr><tr><td>0</td><td>1.183</td></tr><tr><td>−5</td><td>0.267</td></tr><tr><td>−17</td><td>0.125</td></tr></table></td></tr>
<tr><td>$T_{\text{glass transition}}$ ($T_{g1/2}$) [°C]</td><td>−61.5, −72.6 (rerun) (DSC @ 10 °C/min)[18], labile form does not readily freeze and turns to glass instead[33], −72[42], NG (both forms) tends to supercool[59]</td></tr>
<tr><td>$T_{\text{phase transitions}}$ [°C]</td><td>Freezing very pure NG usually transforms it into labile form of crystals, samples with lower purity usually crystallize as stable form[32], labile form produced by mixing NG with wood meal or pulverized glass and cooled to −40 °C with vigorous stirring[32], introducing a crystal of labile form into cooled NG induces crystallization of labile form[32], stable crystalline form produced by mixing NG with wood meal and AN or $NaNO_3$[32], readily melting crystalline NG and allowing it to solidify results in same crystalline form prior to melting[32], labile form converts to stable form after 1–2 week storage (Hibbert)[32], labile – stable form conversion does not occur readily; labile-form NG did not convert to stable-form NG after storage @ 4 months @ 0 °C (Hackel)[32], formation of labile-form promoted by addition of urethane, polyurethane, collodion, nitrocotton, cyclonite, tetryl, dinitrobenzene, centralite I, centralite II[32], admixtures of siliceous earth, TNB or TNT promote formation of stable form[32], cooling to −20−−60 °C and seeding with crystals of one form results in crystallization of the seed form[33], if solid NG is melted to just above its mpt. and then cooled, it will solidify in the form in the premelting form[33], pure NG freezes to form rhombic crystals (stable form), but under certain conditions triclinic crystals form[55], labile gradually converts to stable form within 2 weeks[55], gradual conversion of labile to stable form after 1–2 weeks (heat of conversion = 28 cal/g)[20], technical NG freezes more readily than pure NG and usually in the stable form[59], pure NG is harder to freeze than technical NG but always solidifies in the labile form[59], labile NG converts to stable NG if mixture is agitated with a glass rod[59], labile form converts to stable form gradually within 1–2 weeks on sitting[59], NG has two crystalline modifications: α (triclinic) and β (orthorhombic)[66]</td></tr>
<tr><td>$T_{\text{b.p.}}$ [°C]</td><td>145 (dec.)[9], >180 °C (boiling begins, dec.)[32], not determined due to dec.[32], 180 @ 50 mm Hg[32, 33, 55, 69], 125 @ 2 mm Hg[32, 33, 55, 69], dec.[35], 245 ± 5 @ 760 mm Hg (most probable value)[33], gradual dec. @ 145 °C with ebullition of gaseous products so appears to boil[55], 145 (apparent, but actually represents T of nonexplosive dec. which is vigorous enough to resemble boiling)[20], true boiling occurs @ reduced pressure: 125 °C @ 2 Torr and 180 °C @ 5 Torr[20], some dec. even occurs under high vacuum boiling[20], >180 (with dec.)[69], 189.5 (endo, onset), 192.1 (endo, peak max) (DSC 10 K/min)[70]</td></tr>
</table>

<table>
<tr><td>$T_{dec.}$ [°C]</td><td>143[2], 145–150 (dec.)[16], begins to dec. as low as 50–60 °C with rapid dec. @ 135 °C (reddish color)[33], 149 (TGA midpoint)[43], 170 (onset), 196 (peak max) (DSC @ 5 °C/h, hermetic sealed Al pans)[47], 197.4 (onset), 199.9 (peak max), 202.1 (end T) (DSC @ 10.0 K/min, pinhole cover)[48], 145 (gradual with ebullition of gaseous products)[55], >180 (boils with dec.)[69], 197.4 (exo, onset), 199.9 (exo, peak max) (DSC 10 K/min)[70]

Nonisothermal TG data[70]:

<table>
<tr><th rowspan="2">β/K min^{-1}</th><th rowspan="2">T_{ot}</th><th rowspan="2">T_i</th><th colspan="2">Mass loss/%</th><th rowspan="2">L_{max}/% min^{-1}</th><th rowspan="2">T_p/°C</th><th rowspan="2">T_{oe}/°C</th></tr>
<tr><th>Stage 1</th><th>Residue/%</th></tr>
<tr><td>5.0</td><td>145.8</td><td>82.4</td><td>99.63</td><td>0.42</td><td>–20.74</td><td>165.8</td><td>169.2</td></tr>
<tr><td>7.0</td><td>154.9</td><td>83.9</td><td>98.51</td><td>0.38</td><td>–24.79</td><td>177.4</td><td>182.8</td></tr>
<tr><td>10.0</td><td>161.4</td><td>93.2</td><td>99.42</td><td>0.25</td><td>–31.74</td><td>183.8</td><td>185.5</td></tr>
<tr><td>15.0</td><td>171.2</td><td>98.1</td><td>99.41</td><td>0.06</td><td>–55.25</td><td>191.9</td><td>203.1</td></tr>
</table>
T_{ot} = onset T of dec., T_{oe} = onset T of end dec., T_i = initial T for thermal dec., T_p = peak T of mass loss rate, Stage 1 = from initial T to end T od DTG peak, L_{max} = max. mass loss rate</td></tr>
<tr><td>ρ [g cm^{-3}]</td><td>1.6009 (@ 288 K)[1], 1.591 (liquid @ 25 °C)[2, 9], 1.596 (liquid @ 20 °C)[2, 9, 55], 1.600[3], 1.60 (loading ρ @ 25 °C)[15, 16], 1.596 (@ TMD)[20], sp. gr. = 1.591 (@ 25°)[16], d_4^{20} = 1.5931[32], sp. gr. = 1.614 @ 4 °C[32, 69], sp. gr. = 1.600 @ 15 °C[32, 69], sp. gr. = 1.591 @ 25 °C[32], sp. gr. = 1.5995 @ 15 °C[32], sp. gr. = 1.735 @ 10 °C (stable form)[32], sp. gr. = 1.6009 @ 15 °C[33], sp. gr. = 1.5910 @ 25 °C[33], 1.59 @ 27 °C[35], 1.59[39, 49], 1.596[45], 1.59[51], 1.6[52], sp. gr. = 1.596 (20/15)[20], sp. gr. $d^{20°}_{15°}$ = 1.596[59], 1.6009 @ 15 °C[59], 1.5910 @ 25 °C[59], sp. gr. = 1.735 (frozen NG)[59], 1.59 (liquid @ 25 °C)[62], 1.595[63], 1.60 (liq.)[67], d^{16}_{16} = 1.5985[69], sp. gr. = 1.590 @ 25 °C[69], sp. gr. = 1.5995 @ 15 °C[69], sp. gr. = 1.735 (stable form @ 100 °C)[69]</td></tr>
<tr><td>Heat of formation</td><td>–400 cal/g[9], –90.8 kcal mol^{-1}[10, 20], –1,632 J/g (ΔH_f)[39], –378.3 kJ/mol ($\Delta_f H°$)[45], – 1,633 kJ/kg [2], –1,673.6 kJ/kg[3], 81.7 kcal/mol[17], 400 cal/g[16, 19], 359.8 cal/g[17], 415 kcal/kg (Brunswig)[32], 416 kcal/kg (Kast)[32], 370 kcal/kg (Taylor)[32], 85.3 kcal/mol (–ΔH_f, heat of form., Rinkenbach based on heat of combustion values)[32], –392 cal/g (ΔH_f)[35], –1,632 kJ/kg (ΔH_f, ICT thermochemical database)[36], –371 kJ/mol (ΔH_f)[51], 88.63 kcal/mol (heat of form., ΔH) [59], 362.3 kcal/kg (heat of form., (Q))[59], –392.0 kcal/kg (enthalpy of form.)[38], –113 kcal/mol (calcd.)[67], –356.9 kJ/mol (enthalpy of form., ΔH_f)[69], –90.8 kcal/mol[10]</td></tr>
<tr><td>Heat of combustion</td><td>1,616 cal/g[9, 62], 1,630.4 cal/g (@ C^v)[17], 270.5 kcal mol^{-1} (@ C^v)[17], 1,622.1 cal/g (@ C^p)[17], 368.36 kcal mol^{-1} (@ C^p)[17], ΔH_c = 368.4 kcal/mol (@ C^v, Rinkenbach)[32], ΔH_c = 1,623 kcal/kg (@ C^v, Rinkenbach)[32], ΔH_c = 6,761 J/g[39], –6.72 kJ/g (exptl.)[58], heat of combustion ΔH = 1,622 cal/g[59], 1,623 kcal/kg (@ C^v)[59], 1,541.39 (heat of comb.)[69], 1,529.0 kJ/mol (ΔH_c, heat of comb.)[70]</td></tr>
</table>

	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]	6,099	6,213[4, 69] 1,486 cal/g[16] 1.48 kcal/g[31, 59] 1.59 kcal/g [H_2O (l)][26] 1.48 kcal/g [H_2O (g)][26] 1,485 kcal/kg (calcd., *Naoúm*)[32] 1,455 kcal/kg (calcd., *Kast*)[32] 1,470 kcal/kg (*Escoles*)[32] 1,478 kcal/kg (*Berthèlot*)[32] 1,580 cal (*Brunswig*)[33] 6,671 J/g (calcd., ICT code)[36] 1,487 kcal/kg (@ 1.593 g cm^{-3}, calcd.) [H_2O vapor][38] 6,669 J/g (ΔH_e)[39] 6,675 J/g [H_2O (l)] (calcd., ICT thermodynamic code)[43] 6.18 MJ/kg (calcd., SD method)[61] 161.6 kcal/100 g (@ 1.60 g cm^{-3}, constant volume) [H_2O (l)][63]	6,095 16,00 cal/g[9, 16, 62] 1,486 cal/g (heat of detonation)[9] 1,589 cal/g (@ const. vol.) [H_2O (l)][17] 1,470 cal/g (@ const. vol.) [H_2O (g)][17] 1,486 cal/g [H_2O (g)][20] 1,590 cal/g [H_2O (l)][20] 6,671 [H_2O (l)][13] 6,214 [H_2O (g)][13] 1,472 kcal/kg (@ 1.593 g cm^{-3}) [H_2O vapor][38]

T_{ex} [K]	4,316	4,250[4] 3,270 (@ 1.6 g cm^{-3})[19] 5,730 °C (@ 1.60 g cm^{-3}, calcd., hydrodynamic theory)[19] 3,185 °C (calcd., *Naoúm*)[32] 4,250 °C (calcd., *Kast*)[32] 3,153 °C (*Gody*)[32] 3,005 °C (*Wuich*)[32] 3,470 °C (*Brunswig*)[33] 3,887 (calcd., ICT code)[36] 4,556 (calcd., SD method)[61] 4,645 °C (@ 1.60 g cm^{-3})[63] 4,250 °C[69] 3,750 (@ 1.60 g cm^{-3}; calcd. BKWR)[10] 4,550 (@ 1.60 g cm^{-3}; calcd. BKWS)[10]	4,554 4,177 °C[17] 4,260[10] 4,645 °C[16] ~3,470 °C (calcd./ exptl. not specified)[16] 3,470 °C (@ 1.60 g cm^{-3})[19] 4,577 °C[20] 4,000[31] 3,500[31]
$p_{C\text{-}J}$ [kbar]	23.7	277 (@ 1.592 g cm^{-3}, calcd., K-J)[30] 256 (@ 1.6 g cm^{-3})[19] 124.0 MPa (calcd., ICT code)[36] 260 (@ 1.60 g cm^{-3}, calcd. BKWR)[10] 250 (@ 1.60 g cm^{-3}, calcd. BKWS)[10]	25.6 GPa 253[10, 26] 253 (@ 1.6 g cm^{-3})[19, 31] 253 (@ 1.59 g cm^{-3})[20] 253 (@ 1.592 g cm^{-3})[30] 10,000 atm[20] 0.241 Mbar[62]

VoD [m s^{-1}]	7,850	7,450 (@ 1.6 g cm^{-3})[4] 7,940 (@ 1.60 g cm^{-3}, calcd. BKWR)[10] 8,010 (@ 1.60 g cm^{-3}, calcd. BKWS)[10] 7,440 (@ 1.60 g cm^{-3} (TMD), calcd., R-P method)[29] 7,800 (@ 1.60 g cm^{-3} (TMD), calcd., *Aizenshtadt*)[29] 8,060 (@ 1.60 g cm^{-3}, calcd., hydrodynamic theory)[19] 8,310 (@ 1.593 g cm^{-3}, calcd., K-J)[48] 8,060 (@ 1.60 g cm^{-3}, calcd., K-W eqn.)[53]	7,804 7,630 (@ 1.6 g cm^{-3} loading ρ)[19] 7,650 (@ 1.6 g cm^{-3} loading ρ)[19] 7,700 (@ 1.6 g cm^{-3})[5, 6, 10] 1,600–1,900 (@ 1.6 g cm^{-3}, liquid, glass confinement, 0.39 in charge diameter)[7, 9, 16] 7,700 (@ 1.6 g cm^{-3}, liquid, steel confinement, 1.25 in charge diameter)[7, 9, 16] 7,700 (@ 1.59 g cm^{-3})[12] 7,700 (@ 1.6 g cm^{-3}, when properly initiated)[20] 1,500–2,000 (when improperly initiated)[20] 7,700 (@ 1.60 g cm^{-3})[14, 25, 31] 1,560 (30 mm loading diameter, lead tube, directly detonated by no. 8 detonator)[24] 915 (3.0 mm loading diameter, Al tube, directly detonated by no. 8 detonator)[24] 1,130 (9.0 mm loading diameter, Al tube, directly detonated by No. 8 detonator)[24]

			7,800 (28 mm loading diameter, Plexiglass tube, detonated by no. 8 detonator, 15 g tetryl as transmitted detonation pellets)[24] 8,560 (40 mm loading diameter, #12 antirust Al tube, detonated by no. 8 detonator, 20 g tetryl as transmitted detonation pellets)[24] 6,970 (30 mm loading diameter, #12 antirust Al tube, detonated by no. 8 detonator, 20 g tetryl as transmitted detonation pellets)[24] 5,870 (20 mm loading diameter, #12 antirust Al tube, detonated by no. 8 detonator, 20 g tetryl as transmitted detonation pellets)[24] 7,700 (@ 1.50 g cm^{-3})[26] 29,200 ft/s (@ 1.59 g/mL)[50] 8,000 (@ 1.60 g cm^{-3})[53] 9,150 (stable form, steel tube of 22 mm diameter, no. 6 detonating cap)[59] 7,649 (@ 1.60 g cm^{-3}, D_i) (D_i = ideal detonation velocity)[61] 6,741 (@ 1.60 g cm^{-3}, D_f) (D_f = detonation velocity for critical detonation diameter)[61] 7,700 (@ 1.60 g cm^{-3})[63]

			VoD ranges from 100–8,000 m/s depending on charge diameter and configuration[69] VoD of NG increases with increasing charge diameter[69] 920 can only be reached with charge diameter <5 mm[69] See additional tables at end of section
V_0 [L kg^{-1}]	782	715 (@ 0 °C)[4] 715.53 L (@ 0 °C, 760 mm Hg, calcd. to T_{ex} of 4,177° = 11,663 L)[17] 715.7 (calcd., *Naoúm*)[32] 715.1 (calcd., *Kast*)[32] Specific volume = 712 L (*Brunswig*)[33] 512 (without H_2O @ 25 °C)[43] 716[59] 71.5 l/100 g (@ 1.60 g cm^{-3}, @ STP)[63] 715.7[69]	714 715[9, 62] 716 [11, 13] 717.7 mL/g[24] 715 mL/g[20]

Luminosity method: VoD = 7,650 m/s, T = 4,000 K, pressure = 250,000 atm[17]
variation of VoD with cartridge diameter, NG powder[53]:

Diameter (cm)	VoD (m/s)	Diameter (cm)	VoD (m/s)
1.9	1,830	10.2	3,290
3.2	2,250	12.7	3,440
5.1	2,610	15.2	–
6.4	–	21.6	3,920
7.6	3,150		

Relationships between detonation velocity and charge configuration and detonator[69]:

Charge medium	Charge diameter (mm)	Detonation condition	Detonation velocity (m/s)
Lead tube	30	No. 8 detonator	1,560
Aluminum tube	3.0	No. 8 detonator	915
Aluminum tube	9.0	No. 8 detonator	1,130
30CrMnSi tube	30	No. 8 detonator	3,780
Glass tube (3.0 mm wall thickness)	22	No. 8 detonator	1,165
Organic glass tube	28	No. 8 detonator, 15 g tetryl booster	7,800
30CrMnSi tube (1.0 mm wall thickness)	37.5	No. 8 detonator, 2 g mercury(II) fulminate booster	8,520
Organic glass tube	25	No. 8 detonator, 50 g tetryl booster	7,410
30CrMnSi tube	22	No. 8 detonator, 75 g tetryl booster	7,760
#12 corrosion-resistant Al tube	40	No. 8 detonator, 20 g tetryl booster	8,560
#12 corrosion-resistant Al tube	35	No. 8 detonator, 20 g tetryl booster	7,830
#12 corrosion-resistant Al tube	30	No. 8 detonator, 20 g tetryl booster	6,970
#12 corrosion-resistant Al tube	25	No. 8 detonator, 20 g tetryl booster	6,100
#12 corrosion-resistant Al tube	20	No. 8 detonator, 20 g tetryl booster	5,870

Data from[69]

H_2O:NG	Detonation condition	Detonation velocity (m/s)
0.75:1	No. 8 detonator, 15 g tetryl booster	6,370
1:1	No. 8 detonator, 15 g tetryl booster	5,520
1.5:1	No. 8 detonator, 15 g tetryl booster	5,150
2:1	No. 8 detonator, 15 g tetryl booster	4,300

<table>
<tr><td>Detonation failure diameter, d_c [mm]</td><td>2 mm (neat NG in glass capillary)[45]

Measurements of d_c and initiation pressure (P_i) on homogeneous explosive[56]:

<table><tr><td>Material</td><td>Form</td><td>ρ_0 (g/cc)</td><td>P_i (kbar)</td><td>d_c (mm)</td></tr><tr><td>NG</td><td>Liq., 20 °C</td><td>1.59</td><td>85</td><td>2.1</td></tr></table>
2.0 mm[61]</td></tr>
<tr><td>Trauzl test [cm^3, % TNT]</td><td>181[7, 9], 185% TNT[14], 590 cc (10 g sample cf. 300 cc for TNT)[16], 590 cc (10 g NG with water tamping)[17, 33], 115% TNT[20], 515–563 cc[25], 390 cc (stable form of NG)[17, 20], 560 cc (labile form of NG)[17, 20], 518 cc (liq. NG)[17, 20], 550 (10 g sample, sand tamping)[33], 550 mL[59], 520[64], 542[64]

Lead block expansion (10 g sample in glass tube)[33]:

<table><tr><td>Sp. gr. @ 20 °C</td><td>Sand tamping</td><td>H_2O tamping</td></tr><tr><td>1.596</td><td>550 cc</td><td>595 cc</td></tr></table>
Lead block expansion values of NG detonated by different detonators[69]:

<table><tr><td>Detonator</td><td>Lead block expansion value (cm)</td></tr><tr><td>1</td><td>190</td></tr><tr><td>2</td><td>225</td></tr><tr><td>6</td><td>460</td></tr><tr><td>8</td><td>590</td></tr></table>
Lead block expansion values of NG detonation[69]:

<table><tr><td>NG phase</td><td>Pure NG (cm^2)</td><td>Sand filling (cm^2)</td><td>Water filling (cm^2)</td></tr><tr><td>Stable crystallite</td><td>–</td><td>380</td><td>540</td></tr><tr><td>Unstable NG crystallite</td><td>–</td><td>390</td><td>525</td></tr><tr><td>Liquid</td><td>–</td><td>390</td><td>530</td></tr></table></td></tr>
<tr><td>Lead cylinder</td><td>18.5 mm upset of lead cylinder when exploded by MF cap[59]</td></tr>
<tr><td>Sand test [g]</td><td>51.5 g (200 g bomb, liquid)[7, 9], 120% TNT[14, 20], 51.5 g sand crushed (cf. 48 g for TNT)[16]</td></tr>
</table>

<table>
<tr><td>Ballistic mortar test</td><td>140% TNT[7, 9, 14, 16]</td></tr>
<tr><td>Ballistic pendulum test</td><td>RDX and PETN are more powerful than NG[20]</td></tr>
<tr><td>Koenen test</td><td>Exploded after 24 s with nozzle plate containing a hole of 24 mm diameter[58]</td></tr>
<tr><td>Initiation efficiency</td><td>Can be fired with a commercial no.1 blasting cap but full power only achieved using no.8 blasting cap[50], rel. insensitive to detonation, requires no. 8 cap to cause complete detonation[59]</td></tr>
<tr><td>Gap test</td><td>Blends of 15% NG and 85% inert salts packed into two 30–32 mm diameter tubes and placed end to end on dry sand at a specific distance apart. Detonation of one tube resulted in detonation of the other tube at the following maximum gaps: NH_4Cl = 25 cm, NaCl = 11 cm, $NaHCO_3$ = 10 cm, $(NH_4)_2SO_4$ = detonation not transmitted even at 0 cm, $(NH_4)_2CO_3$ = detonation not transmitted even at 0 cm, chalk = detonation not transmitted even at 0 cm, talc = detonation not transmitted even at 0 cm[20]</td></tr>
<tr><td>5 s explosion T [°C]
5 s ignition T [°C]
Explosion T [°C]

Initiation T [°C]

Ignition T [°C]
Detonating T [°C]

Thermal ignition T [°C]</td><td>200–205[19], 222[7, 16, 20, 62]

222 (US value)[9, 16, 19, 40], 220–222 (Russian value, explodes)[16, 19]
Explosion T @ various times of exposure (3 mg samples, detonation)[17]: 0.108 s @ 261 °C[17], 0.675 s @ 230 °C[17], 3.75 s @ 211 °C[17], no action @ 205 °C[17], 215–250 (NG dropped onto metal plate; if T>420 °C NG burns gently)[32], 215[33], iron heated to red heat in contact with NG results in explosion[59], explodes on rapid heating to 180 °C[59]

200–205 (bath temperature, @ 20 °C/min heating rate)[32, 40], 155 (calorimetric)[40]
188[34], 200[33]
218[50], detonated by lightning[59], detonates on rapid heating to 200 °C[59]

200[62]</td></tr>
<tr><td>100 °C heat test [% mass loss]</td><td>3.6% in first 48 h[9, 16], 3.5% in second 48 h[9, 16], no explosion in 100 h[9, 16]</td></tr>
<tr><td>Thermal stability</td><td>Gas evolved @ atmospheric pressure, in cc[9]:

<table>
<tr><td>Sample wt. (g)</td><td>1.6</td><td>1.6</td></tr>
<tr><td>T (°C)</td><td>65</td><td>75</td></tr>
<tr><td>Time (h)</td><td>20</td><td>40</td></tr>
<tr><td>Vol. of gas (cc)</td><td>Nil</td><td>Nil</td></tr>
</table>

Stability @ 75 °C (loosely covered weighing dish): 28.0% began to dec. after 12 days[17], 54.0% after 18 days[17], complete dec. of 73.5% after 25 days[17] dec. begins @ 50–60 °C[20], NG is quite stable @ T<50 °C in storage tests over period of years but dec. increases rapidly higher T[20]</td></tr>
</table>

<table>
<tr><td></td><td>
Moles of gas produced/mole compound on heating[27]: 2.54 after 22 h @ 120 °C[27], 3.2 mol after 72 h @ 120 °C[27], 3.55 after 22 h @ 220 °C[27], 3.50 after 72 h @ 220 °C[27], 3.96 after 22 h @ 320 °C[27], 4 after 72 h @ 320 °C[27]

11 cm^3/g gas released @ 100 °C, 16 h, 1 g sample, thermostating with LAVA set-up[40]

Nonisothermal TG data, β = °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.[48]:

<table>
<tr><td>β (°C/min)</td><td>T_{ei} (°C)</td><td>T_p (°C)</td><td>T_{oe} (°C)</td><td>T_b (°C)</td></tr>
<tr><td>5.0</td><td>145.8</td><td>165.8</td><td>169.2</td><td>114.2</td></tr>
<tr><td>7.0</td><td>154.9</td><td>177.4</td><td>182.8</td><td></td></tr>
<tr><td>10.0</td><td>161.4</td><td>183.8</td><td>185.5</td><td></td></tr>
<tr><td>15.0</td><td>171.2</td><td>191.9</td><td>203.1</td><td></td></tr>
</table>

Stable indefinitely @ RT[50], quite stable on storage @ 50 °C for several years[55], rapid dec. @ T>50 °C[55], stable @ T<50 °C, but higher T causes dec. which rapidly increases as T increases[7], dec. with liberation of HNO_3 when steam distilled[59], hydrolysis @ T>80 °C in H_2O[59], stable @ RT but begins to dec. @ T>50 °C[59], converted to acidic compounds after 3–4 days @ 75 °C[69], dec. can be slow if the dec. products are removed[69], in sealed system, NO_x produced during decomposition catalyze the dec. reaction[69], critical T for thermal dec. = 114.2 °C[70]
</td></tr>
<tr><td>Vacuum stability test [cm^3/h]</td><td>
1.6 cc/g/6 h @ 40 °C[9], 11 + cc/g/16 h @ 100 °C[9], 1.6 cc/g/5 h @ 90 °C[16], 11 + cc/g/16 h @ 100 °C[16], 0.519 mL/g @ 90 °C/40 h (1 g sample)[47], 12 ¾ h (time required for >12 cc gas to be produced@ 100 °C, 2.4 g sample)[60]
</td></tr>
<tr><td>Vapor pressure [mm Hg/°C]</td><td>
Vapor pressure values from[9]:

<table>
<tr><td>°C</td><td>mm Hg</td><td>°C</td><td>mm Hg</td></tr>
<tr><td>20</td><td>0.00025</td><td>60</td><td>0.0188</td></tr>
<tr><td>30</td><td>0.00083</td><td>70</td><td>0.043</td></tr>
<tr><td>40</td><td>0.0024</td><td>80</td><td>3.098</td></tr>
<tr><td>50</td><td>0.0073</td><td>90</td><td>0.23</td></tr>
</table>
</td></tr>
</table>

0.00038/20[17], 0.0081/50[17], 0.00025/20[17], 0.00083/30[17], 0.0024/40[17], 0.0072/50[17], 0.0188/60[17], 0.043/70[17], 0.098/80[17], 0.29/93.3[17], 0.0015/20[26], 0.00130/15[17], 0.0177/25[17], 0.00459/35[17], 0.01294/45[17], 0.03587/55[17], dec. begins @ 50–60 °C[17], 580 ppb @ 26 °C (av. value, two different trapping methods)[28], <0.00012 mm Hg @ 25 °C (*Chiaraviglio*)[32], 0.011 mm Hg @ 20 °C (*Naoúm*, dynamic method)[32], 0.036 mm Hg @ 60 °C (*Naoúm*, dynamic method)[32], 0.015 mm Hg @ 20 °C (*Rinkenbach*)[32], 0.060 mm Hg @ 60 °C (*Rinkenbach*)[32], 0.00177 Torr @ 25 °C[49], 740 ppb_v (equilibrium vapor pressure @ 300 K)[54], 5.1×10^6 ppb_v (equilibrium vapor pressure @ 400 K)[54], 2×10^{-4} mm Hg @ 25 °C[57], 0.0060 mm @ 60 °C[59], 0.0013 Torr @ 15 °C[20], 0.0015 Torr @ 20 °C[20], 0.00177 Torr @ 25 °C[20], 0.00459 Torr @ 35 °C[20], 0.0075 Torr @ 40 °C[20], 0.01294 Torr @ 45 °C[20], 0.03587 Torr @ 55 °C[20], 0.06 Torr @ 60 °C[20]

Vapor pressure (*Marshall*, *Peace*)[32, 33, 69]:

Vapor pressure (mm Hg)	*T* (°C)	Vapor pressure (mm Hg)	*T* (°C)
0.00025	20	0.0188	60
0.00038	30	0.043	70
0.0024	40	0.098	80
0.0072	50	0.29	93.3

Vapor pressure according to *Brandner*[32]:

Vapor pressure (mm Hg)	*T* (°C)	Vapor pressure (mm Hg)	*T* (°C)
0.0012	30	0.0047	45
0.0020	35	0.0081	50
0.0030	40		

Saturated vapor pressure (Pa) (statistical and dynamic gas chromatography)[42]: 0.10 @ 25 °C, 0.17 @ 30 °C, 0.49 @ 40 °C, 1.16 @ 50 °C, 2.86 @ 60 °C[42]

Vapor pressures of NG/diethyleneglycol dinitrate mixtures[69]:

Diethyleneglycol dinitrate (%)	Total vapor pressure (mm Hg)			
	10 °C	30 °C	40 °C	50 °C
10	0.0027	0.0186	0.0433	0.1002
20	0.0051	0.0345	0.1159	0.1841
40	0.0093	0.0624	0.1475	0.3314
60	0.0137	0.0874	0.2417	0.6316

<table>
<tr><td>Volatility</td><td>0.11 mg/cm^2/h @ 60 °C[9, 16, 20, 32], 0.153 × 10^{-3} g/cm^2/24 h lost @ 25 °C[15]
Mass loss from 20 g NG in 24 h in an open dish of 70 mm diameter: 0.2% @ 50 °C[17], 1.6% @ 75 °C[17], 10% @ 100 °C[17]
Evaporation rate (20 g sample on 70 mm diameter watch-glass for 24 h, mass loss): 0.04 g (0.2%) @ 50 °C[32], 0.32 g (1.6%) @ 75 °C[32], ~ 2 g (~10%) @ 100 °C[32]
0.1 mg•cm^2•h^{-1} (@ 60 °C)[39], 0.45% mass loss in 10 days @ 20 °C[59], 1.68% mass loss @ 50 °C in 10 days[59]

Slightly volatile[69], 0.11 mg/cm^2/h @ 60 °C[69]

20 g NG in glass tube, 70 mm diameter heated @ different T for 24 h[69]:

<table>
<tr><td>T (°C)</td><td>Volatile (g)</td><td>% of volatile (%)</td></tr>
<tr><td>50</td><td>0.04</td><td>0.2</td></tr>
<tr><td>75</td><td>0.32</td><td>1.6</td></tr>
<tr><td>100</td><td>2.00</td><td>10.0</td></tr>
</table>
</td></tr>
<tr><td>Burn rate [mm/s]</td><td>Not easily flammable[50], unconfined NG in very small quantities burns without explosion[55], very slight confinement of NG causes detonation with a loud noise if exposed to flame[55], ignition of NG with gas flame or hot wire in 20 mm diameter glass tube only partially combusts NG and no explosion occurs[69], igniting preheated NG can causes rapid explosion[69], combustion velocity = ~ 0.075 cm/s up to 0.13 cm/s @ 98 °C under the critical pressure of 320 mm Hg[69], NG can be combusted constantly under 400 mm Hg[69], 0.23 cm/s under standard atmospheric pressure[69]

Combustion velocity and pressure, approx. values from graph[69]:

<table>
<tr><td>P (mm Hg)</td><td>v (cm/min)</td></tr>
<tr><td>200</td><td>5</td></tr>
<tr><td>400</td><td>6</td></tr>
<tr><td>600</td><td>8</td></tr>
<tr><td>800</td><td>13</td></tr>
<tr><td>900</td><td>23</td></tr>
</table>
</td></tr>
<tr><td>Solubility [g/mL]</td><td>Values from[9]: 1% in CS_2 @ ambient T[9], infinite @ 25 °C in ether[9], >100% in 2:1 ether:alcohol @ 25 °C[9], soluble in all proportions in MeOH, acetone, ether, ethyl acetate, amyl acetate, methyl nitrate, ethyl nitrate, nitroglycol, tetranitrodiglycerine, acetic acid, benzene, toluene, phenol, pyridine, xylene, nitrobenzene, p-nitrotoluene, liquid DNT, chloroform, ethyl chloride, ethyl bromide, tetrachloroethylene, dichloroethylene and trimethyleneglycol dinitrate[9]</td></tr>
</table>

Solubility *in* NG of[9]:

Alcohol		DNT		TNT		Water	
°C	%	°C	%	°C	%	°C	%
0	3.5	20	35	20	30	25	0.06
20	5.4						
50	∞						

Solubility *of* NG in[9]:

Water[9, 69]		Alcohol[9]		Trichloroethylene[9]		CCl_4[9]	
°C	%	°C	%	°C	%	°C	%
15	0.16	0	37.5	Rm	22	Rm	2
20	0.18	20	54.0				
50	0.25						

0.173 g/L H_2O @ 20 °C[20], 0.191 g/L H_2O @ 30 °C[20], 0.228 g/L H_2O @ 50 °C, 0.246 g/L H_2O @ 60 °C[20], 37.5 g/100 g EtOH (abs.) @ 0 °C[20], 54 g/100 g EtOH (abs.) @ 20 °C[20], 40 g/100 g 96% EtOH @ 20 °C[20], 20 mL/L CCl_4[20], 20 parts/100 parts trichloroethylene[20], 12.5 g/L CS_2 @ RT[20], hot EtOH and NG are misicible in all proportions[20], NG is miscible in all proportions with Et_2O, acetone, glacial acetic acid, ethyl acetate, benzene, toluene, phenol, nitrobenzene, $CHCl_3$, ethylene chloride and nitric esters such as glycol dinitrate[20], 100 g/35 g dinitrotoluene @ 20 °C[20], hardly miscible with H_2O[32], 1.6 g dissolves in 1 L H_2O @ 15 °C[32], 1.8 g dissolves in 1 L H_2O @ 20 °C[32], 2.5 g dissolves in 1 L H_2O @ 50 °C[32], soluble in most common organic solvents[32], NG acts as a good solvent[32], completely miscible in all proportions @ RT with MeOH, ethylacetate, anhydrous CH_3COOH, benzene, toluene, xylenes, phenol, nitrobenzene, nitrotoluenes, pyridine, $CHCl_3$, dichloroethane[32, 33], hot absolute EtOH, PrOH, iPrOH and amyl alcohol mix with NG in all proportions[33], 37.5 g dissolved in 100 g abs. EtOH @ 0 °C[33], 54.0 g dissolves in 100 g abs. EtOH @ 20 °C[33], NG dissolves aromatic nitro compounds such as DNT or TNT in all proportions when warm[33], 100 g NG dissolves 3.4 g EtOH @ 0 °C[33], 100 g NG dissolves 5.5 g EtOH @ 20 °C[33], 1.8 g dissolves in 1 L H_2O @ 20 °C[33], aqueous solubility = 1,950 mg/L @ 25 °C[49], slightly soluble in CCl_4[50], very soluble in acetone, Et_2O, EtOH and MeOH[50], 1.95 g/L in H_2O @ 25 °C[52], practically insoluble in cold water[55], soluble in EtOH[55], miscible in all proportions with organic solvents and nitric esters[55], 1,800 mg/L in H_2O @ 25 °C[57]

Solubility of NG in EtOH/H_2O mixtures[32, 69]:

Solvent	T (°C)	NG (g) dissolved in 100 cm^3 solvent
Abs. EtOH	0	~ 30
Abs. EtOH	20	~ 43
96% EtOH	20	31.6
50% EtOH	20	1.8
25% EtOH	20	0.7

NG is miscible in any proportions @ RT with MeOH, acetone, Et_2O, amyl acetate, acetic ether, glacial acetic acid, benzene, toluene, xylene, phenol, pyridine, nitrobenzene, $CHCl_3$ and CH_2Cl_2[59], insoluble in glycerin[59], poorly soluble in EtOH @ RT but miscible in all proportions @ elevated T[59], solubility of NG in EtOH decreases with increasing dilution of EtOH and is poorly soluble in 50% EtOH and precipitates out of soln. at high dilutions[59], poorly soluble in CS_2[59], readily dissolves nitro compounds[59], NG forms low-melting eutectic mixtures with many common nitro compounds[59], NG is readily miscible with many nitric esters[59], solubility in H_2O: 0.14 parts per 100 parts H_2O @ 25 °C, 0.24 parts in 100 parts H_2O @ 60 °C[59], slightly soluble in water[69], 1.0 g/L in 8% aqueous sodium carbonate solns.[69], misible with MeOH, ethyl acetate @ RT[69], 20 parts NG dissolve in 100 parts trichloroethylene[69], almost insoluble in tetrachloroethylene and pentachloroethane[69], solubility in EtOH depends on T and water content: solubility increases with increasing T, NG is miscible with 96% or anhydrous EtOH @ 50 °C[69], slightly soluble in polyols[69], partially soluble in propanol, isopropanol and pentanol @ RT and become miscible @ 90–100 °C[69], 20 g/100 g ethylene glycol @ 200 °C[69], 12 g/100 g ethylene glycol @ 80 °C[69], very low solubility in glycerol[69], soluble in 65% acetic acid[69], insoluble in CS_2[69], slightly soluble in gasoline, crude oil, kerosene, paraffin oil, lubricants, petrolatum oil and other aliphatic hydrocarbons[69], miscible with vegetable oils[69], slightly soluble in ammonia, NaOH, KOH aqueous solns.[69], highly soluble in conc. sulfuric acid[69], miscible with anhydrous nitric acid[69]

Solubility in aliphatic hydrocarbons[69]:

Solvent	*T* (°C)	Solubility (g/100 g)
Crude oil	20	~ 1.5
	80	~ 6.0
Gasoline	20	~ 2
	80	~ 6
Refined oil	20	~ 4
	80	~ 9
Olive oil	20	20
	100	25
Castor oil	20	26
	100	30

Solubility of NG in water[69]:

T (°C)	g NG/100 g water
10	0.14
20	0.15
30	0.16
40	0.18
50	0.21
60	0.25

Solubility in sodium carbonate soln. @ 20–22 °C[69]:

Na_2CO_3 (%)	NG in aq. phase		NG content after 3 h shaking and Et_2O extraction (%)
	after 1 h shaking	after 3 h shaking	
1.39	0.10	0.12	0.10
4.95	0.05	0.06	0.03
10.31	0.02	0.05	0.01

<table>
<tr><td>Viscosity [poises]</td><td>Values from[9]:

<table><tr><td>°C</td><td>Centipoises</td></tr><tr><td>10</td><td>69.2</td></tr><tr><td>20</td><td>36.0</td></tr><tr><td>30</td><td>21.0</td></tr><tr><td>40</td><td>13.6</td></tr><tr><td>50</td><td>9.4</td></tr><tr><td>60</td><td>6.8</td></tr></table>
0.288 @ 20 °C[17], 0.360 @ 20 °C[17], 0.0938 @ 50 °C[17], 0.36 cP @ 20 °C[20], 0.21 cP @ 30 °C[20], 0.094 cP @ 50 °C[20], 0.068 cP @ 60 °C[20], 57.38 cP[32], 1.033 @ 5.1 °C[32], 0.352 @ 20.0 °C[32], 0.0875 @ 55.0 °C[32], viscosity: H_2O < NG << glycerine[32], 37.8 cP @ 20 °C (*de Kreuk*)[32], 35.5 cP @ 20 °C (*Rinkenbach*)[32], 0.36 @ 20 °C[55], 0.360[59]

Viscosity (units not given)[69]:

<table><tr><td>T (°C)</td><td>Viscosity (η)</td></tr><tr><td>5.1</td><td>1.033</td></tr><tr><td>20.0</td><td>0.352</td></tr><tr><td>55.0</td><td>0.0875</td></tr></table></td></tr>
<tr><td>Dielectric constant, ε_{20}</td><td>10.25[32], 19.25[69]</td></tr>
<tr><td>Dipole moment, μ [D]</td><td>3.82[32], 3.82 (pure)[69], 3.16 (soln. in benzene)[69], 2.56 (in hexane)[69], 2.88 (in tetrachloromethane)[69]</td></tr>
<tr><td>Heat of evaporation [kcal/mol]</td><td>ΔH_v = 19.17 (Brandner, calcd.)[32], ΔH_v = 20.64 @ 100 K (*Roginskii*, calcd.)[32], ΔH_v = 20.38 @ 140 K (*Roginskii*, calcd.)[32], ΔH_v = 20.11 @ 180 K (*Roginskii*, calcd.)[32], evaporation enthalpy = 79.1 kJ/mol[42]

Data from[69]

<table><tr><td>T (K)</td><td>Enthalpy of vaporization, ΔH (kJ/mol)</td></tr><tr><td>100</td><td>86.36</td></tr><tr><td>140</td><td>85.27</td></tr><tr><td>180</td><td>84.14</td></tr></table></td></tr>
</table>

<table>
<tr><td>Heat of crystallization [cal/g]</td><td>33.2 (stable form)[32, 59], 5.2 (labile form)[32, 59]

33.2 (stable form, formation of rhombic crystals)[20], 5.2 (labile form, formation of glass triclinic crystals)[20]

Data from[69]

<table><tr><td>Phase</td><td>Heat of crystallization (J/g)</td></tr><tr><td>Stable NG</td><td>138.91</td></tr><tr><td>Unstable NG</td><td>21.76</td></tr><tr><td>Stable NG transformed from unstable NG</td><td>117.20</td></tr></table></td></tr>
<tr><td>Heat of transformation [cal/g]</td><td>Liquid → labile form = 5.2[9], labile form → stable form = 28.0[9, 32, 59], liquid → stable form = 33.2[9]</td></tr>
<tr><td>Hygroscopicity</td><td>0.06% @ 30 °C with 90% RH[9], moderately hygroscopic and presence of moisture increases decomposition[50], nonhygroscopic[7], 0.12% in 24 h @ 100% RH[59]</td></tr>
<tr><td>Radiation sensitivity</td><td>Data obtained from explosives after exposure to gamma radiation[62]:

<table><tr><td>Weight of sample (g)</td><td>1</td></tr><tr><td colspan="2">Vol. of gas produced (mL/g) after:</td></tr><tr><td>10 days</td><td>2.5</td></tr><tr><td>20 days</td><td>5.0</td></tr><tr><td>30 days</td><td>7.5</td></tr><tr><td>40 days</td><td>9.0</td></tr><tr><td>50 days</td><td>10.8</td></tr><tr><td>90 days</td><td>–</td></tr><tr><td>Total irradiation time (days)</td><td>56</td></tr></table>
NG irradiated at ambient T using 0.41 MeV $^{198}_{79}$Au γ-rays; volumes of gas produced measured during and after irradiation, amount of gas evolved as function of gamma dose[68]:

<table><tr><td>Gamma energy absorbed, 10^7 R</td><td>Gas evolved (mL/g) @ STP</td></tr><tr><td>1</td><td>2.5</td></tr><tr><td>2</td><td>5</td></tr><tr><td>3</td><td>6.5</td></tr></table></td></tr>
</table>

<table>
<tr><td></td><td>Critical doses and T to initiate NG by pulsed high-energy electrons,
[a] estimated 50% initiation dose[68]:

<table>
<tr><td>Explosive</td><td colspan="2">Critical dose (J/g)</td><td colspan="2">Ignition T (°C)</td></tr>
<tr><td></td><td>Calcd.</td><td>Exptl.[a]</td><td>Calcd.</td><td>Exptl.</td></tr>
<tr><td>NG</td><td>90.4</td><td></td><td>255</td><td>215–218</td></tr>
</table>

Starts to dec. under UV irradiation within 1–2 min and stops dec. in 2–3 days[69], instantly detonates on irradiation with 900 J of UV radiation @ 100 °C[69], very sensitive to γ-rays and decomposes under γ-ray irradiation[69]</td></tr>
<tr><td>Compatibility</td><td>Hydrolysis with acid: 10 days @ 22 °C <0.002% [9], 5 days @ 60 °C 0.005% [9], dec. by conc. sulfuric acid[20], rapid dec. by aq. NaOH soln. if EtOH is added[20], slight hydrolysis occurs with H_2O producing <0.02% acidity in 10 days @ 22 °C or 0.05% acidity in 5 days @ 60 °C[20], NG does not cause significant corrosion of metals[20], rust increases dec. of NG[20], presence of more than traces of free acid causes NG to be unstable with dec. within a few days[20], moderately hygroscopic and presence of moisture increases dec.[50], contact with free acids increases dec.[50], does not cause significant corrosion of metals[55], traces of free acid makes NG unstable with respect to dec.[55], dec. in acids[59], readily saponified by caustics[59], stability is affected by trace impurities especially metals[69], mixture of 0.3 g NG and 5% nitric acid in sealed glass tube explodes in 6 h[69], dec. starts in 30 h if water content >0.01% and in 2 h if 1.5% water content[69]</td></tr>
<tr><td>ΔH_{melt} [J/g]</td><td>−55.6 (absorption, unreliable value due to evaporation at low heating rates)[48]</td></tr>
<tr><td>$\Delta H_{dec.}$ [J/g]</td><td>24.8 (heat release, unreliable value due to evaporation at low heating rates)[48], −6.37 kJ/g (max heat of dec., calcd. CHEETAH)[58], 0.012 kJ/g (heat value – heat of dec., calcd. CHEETAH)[58], 5.6 kJ/mol (ΔH_d, heat of dec.)[70]</td></tr>
<tr><td>Diffusion coefficient (air) [cm^2/s]</td><td>0.070[49]</td></tr>
<tr><td>Diffusion coefficient (water) [cm^2/s]</td><td>6.95×10^{-6}[49]</td></tr>
<tr><td>Log K_{ow}</td><td>1.62[49, 57], 1.77[49], 1.62 @ 25 °C[52]</td></tr>
<tr><td>Log K_{oc}</td><td>2.77[49], 1.66[49]</td></tr>
<tr><td>Biodegradation</td><td>Readily undergoes aerobic biodegradation[49]</td></tr>
<tr><td>Refractive index</td><td>$n^{D}_{20} = 1.4732$[9, 20, 55, 69], $n^{D}_{25} = 1.4713$[9], $n^{21.2}_{D} = 1.472$[69]</td></tr>
<tr><td>Rifle bullet impact test</td><td>100% explosions in trials[9], explodes on bullet impact[59]</td></tr>
<tr><td>Specific heat [cal/g/°C]</td><td>0.356 (liquid)[9], 0.315 (solid)[9], 0.356 @ 35–200 °C[20], 1.49 J/g[69], 1.317 J/g (crystal, stable form)[69], 1.318 J/g (liquid NG)[69]</td></tr>
</table>

82.1 °C KI test [min]	10 +[9]
Fragmentation test	Fragmentation test, 20 mm HE, Mark 1, projectile, total no. of fragments for NG = 22[9]
Heat of crystallization [cal/g]	
Flash point [°C]	200–205[59]

	Nitroglycerine[22, 23]†	**β-NG (stable modification)[66]**
Chemical formula	$C_3H_5N_3O_9$	$C_3H_5N_3O_9$
Molecular weight [g mol^{-1}]	227.09	227.09
Crystal system	Orthorhombic	Orthorhombic
Space group	*P n a* 2_1 (no. 33)	*P n a* 2_1 (no. 33)
a [Å]	8.900(2)	8.900(3)
b [Å]	13.608(3)	13.608(3)
c [Å]	6.762(2)	6.762(2)
α [°]	90	90
β [°]	90	90
γ [°]	90	90
V [Å^3]	819.0	
Z	4	4
ρ_{calc} [g cm^{-3}]	1.846	1.842
T [K]	153	
	Crystals grown from supercooled ether soln.	Crystals grown from supercooled ethereal soln. @ −3 °C

† Two crystalline forms are known: (i) glassy, labile, triclinic and (ii) stable, orthorhombic[17]; pure NG freezes to form dipyramidal rhombic crystals (stable form)[20], under some conditions, glass triclinic crystals are formed[20]; crystals of labile form are triclinic[59, 65], crystals of stable form are bipyramidalrhombic[59], exists in two crystalline modifications: α- (triclinic) and β- (orthorhombic).[66]

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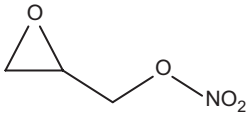
Nitroglycide

Name [German, acronym]: Glycidol nitrate, 2-oxiranylmethyl nitrate, glycidyl nitrate [nitroglycid]

Main (potential) use: Synthetic precursor

Structural formula:



	Nitroglycide		
Formula	$C_3H_5NO_4$		
Molecular mass [g mol^{-1}]	119.08		
Appearance at RT			
IS [J]	2 Nm[2], 10–20 cm (2 kg mass)[3], 10–20 cm (2 kg mass, average height to cause detonation)[6]		
N [%]	11.76		
$\Omega(CO_2)$ [%]	–60.5		
$T_{b.p.}$ [°C]	94 @ 20 mm Hg[3, 4, 6], dec. if boiled under normal pressure @ 174–175[3, 4], 174–175 (boils and decomposes under atmospheric pressure)[6]		
$T_{dec.}$ [°C]	195–200[2]		
ρ [g cm^{-3}]	1.3186 (@ 293 K)[1], sp. gr. = 1.332 (@ 20 °C)[3, 4], 1.332 @ 20 °C[6]		
Heat of formation			
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]		824 kcal/kg[3] 3,447.62[6]	
T_{ex} [K]			
$p_{C\text{-}J}$ [kbar]			
VoD [m s^{-1}]			
V_0 [L kg^{-1}]			

Trauzl test [cm^3, % TNT]	430 cm^3 (H_2O tamping)[3, 6], 430 cc (10 g sample, H_2O tamping, no. 8 detonator)[4], 310 cm^3[5]
5 s explosion *T* [°C] Explosion *T* [°C]	195–200[3, 6], 195–200 (on rapid heating)[4]
Solubility [g/mL]	Slightly soluble in cold H_2O (5 g in 100 mL H_2O @ 20 °C)[3, 4, 6], miscible in all proportions with EtOH[4], Et_2O[4], acetone[4], ethyl acetate[4], NG[4]
Hygroscopicity	Not hygroscopic[4]
Compatibility	Hydrolyzes in boiling water[6]

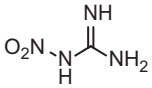
[1] L. T. Eremenko, A. M. Korolev, *Russ. Chem. Bull.*, **1967**, *16*, 1104–1106.
[2] R. Meyer, J. Köhler, A. Homburg, *Explosives*, 7th edn., Wiley-VCH, Weinheim, **2016**, pp. 233–234.
[3] T. Urbański, Ch. 4 in *Chemistry and Technology of Explosives*, *vol. II*, **1965**, Pergamon Press, Oxford.
[4] T. L. Davis, *The Chemistry of Powder and Explosives*, *vol. 2*, **1943**, John Wiley and Sons Inc., New York.
[5] M. Jafari, M. Kamalvand, M. H. Keshavarz, S. Farrashi, *ZAAC*, **2015**, *641*, 2446–2451.
[6] J. Liu, *Nitrate Esters Chemistry and Technology*, Springer, **2019**.

Nitroguanidine

Name [German, acronym]: 2-Nitroguanidine, guanylnitramine, picrite, [nitroguanidin, G-Pulver, G-Salz, NQ, NGu]

Main (potential) use: Insensitive (high) explosive[57], propellant ingredient in triple-base propellants, reduced-erosion gun propellants, component of mixtures for mortar bombs in the WW-I[50], in low-cost large diameter insensitive high explosives[57], low erosion insensitive gun propellants[57], ingredient in gun propellants[19], ingredient of flashless propellants[87]

Structural formula:



	NQ
Formula	$CH_4N_4O_2$
Molecular mass [g mol^{-1}]	104.07
Appearance at RT	NQ exists in two forms: (i) α-form and (ii) β-form[50] (i) α-form: commonly used in explosives, long, flat, thin, lustrous needles if recryst. from H_2O, obtained by dissolving guanidinium nitrate in conc. H_2SO_4 then soln. poured into H_2O[50] (ii) β-form: produced in mixtures with α-form in variable amounts, fern-like clusters of small, thin, elongated plates if recryst. from H_2O, obtained by nitration of guanidinium sulfate/ammonium sulfate mixture which results from the hydrolysis of dicyanamide by sulfuric acid[50] Colorless, hollow needles with length:diameter ratio of ~ 10 with low-bulk density (LBD) on crystallization from aqueous solution[57], colorless, spherical crystals with high-bulk density (HBD) on recrystallization from ethylene glycol, DMF or DMSO[57], white crystalline powder which may be yellow when solid[61], colorless crystals or white solid[10] Needles (length = 30–70 µm, thickness = 3–6 µm, LBD = low-bulk density)[73], platelets (median diameter = 60 µm, HBD = high-bulk density)[73], spherical form (median diameter = 250 µm, SHBD = spherical high bulk density)[73], needles, prisms (α-form, usual stable form, from H_2O)[82], colorless polycrystalline solid[19]

IS [J]	>50 Nm[32, 68, 73], 9.22 (1st reaction)[7, 51], 43.45 (sound)[7, 51], 47 cm (2 kg mass, 20 mg sample, B.M.)[10, 11, 13], 26 in (2 kg mass, 7 mg sample, P.A.)[10, 11, 13], 177 cm (2.5 kg hammer)[17], 47 cm (2 kg, B.M.)[18, 21] 26 in (1 lb mass, P.A.)[18], H_{50} >320 cm (tool type 12)[19], H_{50} >320 cm (tool type 12B)[19], FOI = 100–105 (Rotter apparatus)[21], >320 cm (ERL-LASL, type 12)[21], H_{50} = >177 cm (5 kg mass, tool type 12)[30], IS_{LL} = 5.0 m[20], IS_{A50} = 9.0 m[20], 27.8 in (P.A.)[33], >320 cm (NEDED)[45], >320 cm (NOL)[45], >320 cm (LANL)[45], >49 Nm[48], >50 (BAM)[57], >320 cm (50% point, NQ LBD, type 12 tool, 2.5 kg mass, sandpaper)[74], A_{d1} = 0%, A_{d2} = 0%, LL = 5.0 m, $A_{50\,d1}$ = 9.0 m, $A_{50\,d2}$ = 5.0[81], ≥77.6 ft-lb/in^2[83]
FS [N]	>360[21, 32, 68, 73], $P_{fr.LL}$ = 1,150 MPa[20, 81], $P_{fr.50\%}$ = 1,250 MPa[20, 81], >355 (BAM)[57], unaffected by steel shoe (friction pendulum test)[13, 18], unaffected by fiber shoe (friction pendulum test)[13, 18], wood mallet on stone = 0%[77], wood mallet on softwood = 0%[77], wood mallet on hardwood = 0%[77], ≥722 MPa @ 2.4 m/s[83]
ESD [J]	$E_{50\%}$ = 0.60 ± 0.10 (Bruceton)[46], $E_{50\%}$ = 0.80 ± 0.13[46], 4.5[68], 0.5[83]
N [%]	53.84
Ω(CO_2) [%]	−30.7
$T_{m.p.}$ [°C]	220–257[1], 232[13, 18, 72], 257[14] (depends on heating rate[18]), 246–247 (with dec.)[30], 232 (if temp. is raised at moderate rate, values between 220 and250 have been obtained)[28], 232 (for α- and β- forms with slow heating)[50], 220–250 (values in this range have been obtained depending on the heating rate)[50, 61], dec. immediately on melting cannot be obtained as liquid[50], 252 (dec.)[57], 245 (with dec.)[59], 232 (with dec. on moderate heating)[61], 239[67], 232[10], 232–250 (with dec.)[71], 238[77], 224.5 (dec., Mettle mpt. apparatus @ 1 K/min beginning 10 K beneath the mpt.)[79], 240–250 (melting is usually preceded by dec.)[19], dec. without melting[87]
$T_{phase\ transition}$ [°C]	β-NG can be converted to α-NG by dissolving in conc. sulfuric acid and precipitating by addn. of water[18], β-NG can be converted to α-NG by dec. of the nitrate or hydrochloride formed by β-NG[18], some β-NG forms when α-NG is decomposed by heat[18], α- and β- cryst. forms reported[87] β-form $\xrightarrow{\textit{dissolving in conc. } H_2SO_4 \textit{ and pouring soln. into } H_2O}$ α-form [50] β-form (usual stable form) converted to α-form by dissolving in conc. sulfuric acid followed by pouring into iced water[82]
$T_{dec.}$ [°C]	239 (dec. on melting)[18], 246–247 (melting with dec.)[30] Heating rate of 8 °C/min: T_{idb} = 224.0, T_w = 225.9, T_{max} = 229.4[31] Heating rate of 16 °C/min: T_{idb} = 230.5, T_w = 232.3, T_{max} = 240.0[31], $T_{cr.}$ = 200–204[31] 403 K (DTA onset)[51], 245–250 (dec, onset)[73], 257 (onset, DSC)[68], 225–250 (α-form, usual stable form, depends on heating rate)[82], reported to dec. @ T between 220–257 °C[87], dec. without melting, $T_{dec.}$ depends on heating rate[87]

ρ [g cm^{-3}]	0.91 (@ 293 K) (bulk density)[2], 1.72 (crystal)[13, 72], 1.775[14], 1.759 (crystal @ 193 K)[5], 1.715 (crystal)[18], 1.81[18], needle crystals (bulk ρ) = ~ 0.3 g/cm^3[27], spherical-type crystals (bulk ρ) = 0.9–1.0 g / cm^3[27], 1.55 (nominal)[30], bulk ρ of NQ crystallized from H_2O as needles = 0.17 g cm^{-3}[29], bulk ρ of NQ crystallized from *N*,*N*-DMF (spherical crystals formed) = 0.59 g cm^{-3}[29], sp. gr. = 1.81[28], 1.750 (@ 298 K)[57], 1.72[59], 1.76[62, 77], 1.71[63], 1.81 (@ TMD)[18], 1.55–1.75 (nominal)[18], 0.95 (@ 3,000 psi)[18], 1.77[68], 0.2–0.3 (gravimetric density of NQ crystals obtained from water)[71], 1.78 (X-ray)[73], 1.77 (floating density)[73], 0.3 (LBD, needles, triple base propellants)[73], 0.9 (HBD, platelets, rocket motors)[73], 1.0 (SHBD, spherical form, IHE)[73], 1.78 (X-ray)[19], 1.77 (@ 25 °C, direct measurement)[19], 1.70 (pressed @ 20,000 psi)[19], 0.3 (hand packed density)[87], 1.78 (true density)[87], 0.96 (bulk density, pouring hot, saturated aqueous NQ soln. into MeOH)[87]
Heat of formation	–94 kJ/mol[3], –23.6 kcal/mol (ΔH_f @ 1 atm and 298 K)[30], –20.29 kcal/mol (heat of form., $\Delta H°_f$)[18, 19], –98.7 kJ/mol (ΔH_f)[30], –23.6 kcal/mol[15, 30], –22.1 kcal/mol[21], –20.1 kcal mol^{-1}[12], – 893 kJ/kg (ICT thermochemical database)[4], –227 cal/g[13], –86.61 kJ/mol (enthalpy of form.)[73], 177.6 kcal/kg[70], –93 kJ/mol ($\Delta_f H°$)[68], –92 kJ/mol (ΔH_f)[62], –92.4 kJ/mol (ΔH_f)[44], –86 kJ/mol (ΔH_f)[57], –22 ± 0.59 kcal/mol (ΔH_f^{298}, calcd. based on ΔQ_c value)[79], –23.58 kcal/mol (ΔH_f)[79], –21.86 kcal/mol (ΔH_f)[79], 23.96 kcal/mol (–ΔH_f (heat of form. @ standard conditions))[85]
Heat of combustion	1,995 kcal/kg[13, 28, 34, 72], 210.4 kcal/mol (@ C^P)[18], 2,023 kcal/kg (@ C^V)[70], ΔQ_c = 210 ± 0.59 kcal/mol (exptl.)[79], ΔQ_c = 211.6 kcal/mol[79], ΔQ_c = 209.9 kcal/mol[79], ΔQ_c = 209.2 kcal/mol[79], heat of comb. = 207.15 kcal/mol (@ 1 atm)[84], $\Delta H°_c$ = –210.4 kcal/mol[19], 210 kcal/mol (heat of comb. @ constant volume)[87] exptl. heat of combustion data[85]:

–$\Delta U_{B/M}$ (cal/g)	–ΔU_B (kcal/mol)	–ΔU_R (kcal/mol @ 1 atm and constant vol.)	–ΔH_R (kcal/mol @ 1 atm and constant pressure)
2,005.51 ± 1.63	2,08.72	208.33	207.15

	Calcd. (EXPLO5 6.03)	Lit. values	exptl.

$-\Delta_{ex}U°$ [kJ kg^{-1}]	3,490	3,815 (calcd., K-J)[12] 2,553 (calcd., K-W)[12] 3,815 (calcd., mod. K-W)[12] 3,198 (calcd. thermochem.)[27] 3,071 J/g (calcd., ICT code)[4] 405.7 kJ/mol ($\Delta_{ex}H$)[57] 3.898 kJ/g ($\Delta_{ex}H$)[57]	721[13, 72] 1.06 kcal/g [H_2O (l)][18, 30] 880 cal/g [H_2O (g)][18, 30] 3,071 [H_2O (l)][32] 2,730 [H_2O (g)][32] 721 kcal/kg[28]
T_{ex} [K]	2,505	~2,098 °C[28] 1,385 (@ 1.78 g cm^{-3}, calcd.)[34] 2,418 (calcd. thermochem.)[27] 2,098 °C (@ 0.20 g cm^{-3}, calcd. value based on exptl. data)[50] 2,335 (calcd., ICT code)[4] 2,835 (@ 1.774 g cm^{-3}, calcd., CHEETAH 2.0)[68] 2,811 (@ 1.77 g cm^{-3})[73] 2,064 (@ 1.76 g cm^{-3}, $\Delta H_f = -92.3$ kJ/mol, calcd., JAGUAR)[80] 2,090 (@ 1.78 g cm^{-3}, calcd. BKWR)[15] 2,130 (@ 1.72 g cm^{-3}, calcd. BKWR)[15] 2,210 (@ 1.62 g cm^{-3}, calcd. BKWR)[15] 2,260 (@ 1.55 g cm^{-3}, calcd. BKWR)[15]	2,098 °C[18]

		2,740 (@ 1.78 g cm^{-3}, calcd. BKWS)[15] 2,760 (@ 1.72 g cm^{-3}, calcd. BKWS)[15] 2,790 (@ 1.62 g cm^{-3}, calcd. BKWS)[15] 2,830 (@ 1.55 g cm^{-3}, calcd. BKWS)[15]	
$p_{C\text{-}J}$ [kbar]	28.2	230 (@ 1.69 g cm^{-3}, calcd., K-J)[12] 224 (@ 1.69 g cm^{-3}, calcd., K-W)[12] 230 (@ 1.69 g cm^{-3}, calcd., mod. K-W)[12] 298 (@ 1.78 g cm^{-3}, calcd.)[34] 105.7 MPa (calcd., ICT code)[4] 27.78 GPa (@ 1.774 g cm^{-3}, calcd., CHEETAH 2.0)[68] 27.1 GPa (@ 1.77 g cm^{-3})[73] 30.2 GPa (@ 1.76 g cm^{-3}, $\Delta H_f = -92.3$ kJ/mol, calcd., JAGUAR)[80] 317 (@ 1.78 g cm^{-3}, calcd. BKWR)[15] 292 (@ 1.72 g cm^{-3}, calcd. BKWR)[15] 252 (@ 1.62 g cm^{-3}, calcd. BKWR)[15] 227 (@ 1.55 g cm^{-3}, calcd. BKWR)[15]	245 (@ 1.72 g cm^{-3})[15] 1.20 GPa (@ 0.40 g cm^{-3})[39] 25.8 GPa (@ 1.70 g cm^{-3})[39] 0.160 Mbar[72] 26.8 GPa (@ 1.704 g cm^{-3}, 95 wt.% NQ with 5 wt. % Estane)[19]

		272 (@ 1.78 g cm^{-3}, calcd. BKWS)[15] 250 (@ 1.72 g cm^{-3}, calcd. BKWS)[15] 217 (@ 1.62 g cm^{-3}, calcd. BKWS)[15] 198 (@ 1.55 g cm^{-3}, calcd. BKWS)[15]	
VoD [m s^{-1}]	8,734	7,430 (@ 1.69 g cm^{-3}, calcd., K-J)[12] 7,330 (@ 1.69 g cm^{-3}, calcd., K-W)[12] 7,430 (@ 1.69 g cm^{-3}, calcd., mod. K-W)[12] 8,380 (@ 1.78 g cm^{-3}, calcd.)[34] 5,938 (@ 1.0 g cm^{-3}, calcd., BKWR)[37] 5,521 (@ 1.0 g cm^{-3}, calcd., BKWS)[37] 7,690 (@ TMD, calcd., K-J)[38] 8,270 (@ 1.72 g cm^{-3} (TMD), calcd., R-P method)[38] 8,630 (@ 1.72 g cm^{-3} (TMD), calcd., *Aizenshtadt*)[38] 4,040 (@ 0.6 g cm^{-3}, calcd., K-W eqn.)[65] 8,394 (@ 1.774 g cm^{-3}, calcd., CHEETAH 2.0)[68] 8,329 (@ 1.77 g cm^{-3})[73] 8,770 (@ 1.76 g cm^{-3}, $\Delta H_f = -92.3$ kJ/mol, calcd., JAGUAR)[80]	8,200 (@ TMD)[32] 8,590 (@ 1.78 g cm^{-3})[8, 9, 15] 7,930 (@ 1.62 g cm^{-3})[8, 15] 7,650 (@ 1.55 g cm^{-3})[8, 10, 13–15, 18, 30, 41, 77] 7,980 (@ 1.69 g cm^{-3})[12] 5,360 (@ sp. gr = 1.0)[28] 7,650 (@ sp. gr. = 1.5)[28] 8,100 (@ 1.70 g cm^{-3})[18, 35] 8,160 (@ TMD)[38] 3,490 (@ 0.51 g cm^{-3})[39] 7,380 (@ 1.59 g cm^{-3})[39] 7,720 (@ 1.74 g cm^{-3})[39] 2,990 (@ 0.40 g cm^{-3})[39] 7,360 (@ 1.70 g cm^{-3})[39] 7,650 (@ 1.550 g cm^{-3})[40] 25,100 ft/s (@ 1.6 g/mL)[61] 3,850 (@ 0.6 g cm^{-3})[65] 7,920 (@ 1.56 g cm^{-3})[71]

		8,830 (@ 1.78 g cm^{-3}, calcd. BKWR)[15] 8,580 (@ 1.72 g cm^{-3}, calcd. BKWR)[15] 8,170 (@ 1.62 g cm^{-3}, calcd. BKWR)[15] 7,890 (@ 1.55 g cm^{-3}, calcd. BKWR)[15] 8,530 (@ 1.78 g cm^{-3}, calcd. BKWS)[15] 8,260 (@ 1.72 g cm^{-3}, calcd. BKWS)[15] 7,820 (@ 1.62 g cm^{-3}, calcd. BKWS)[15] 7,520 (@ 1.55 g cm^{-3}, calcd. BKWS)[15] 5,360 (@ 1.0 g cm^{-3})[87]	8,440 (@ 1.64 g cm^{-3})[71] 8,280 (@ 1.69 g cm^{-3}, 95 NQ/5 Estane)[73] 7,060 (@ 1.50 g cm^{-3})[84] 8,280 (@ 1.704 g cm^{-3}, 95 wt.% NQ with 5 wt.% Estane)[19]
V_0 [L kg^{-1}]	925		1,042[16] 1,077[13, 28, 18, 72]

exptl. values @ ρ_0 (absolute charge ρ) = 1.635 g cm^{-3}, η (rel. charge ρ) = 0.918 g cm^{-3}, D_1 (VoD measured @ distance L_1) = 8.25 km/s, D_2 (VoD measured @ distance L_2) = 7.94 km/s, VoD measured using contact foil gages, Q (heat of explosion) = 3,480 kJ/kg, $P_{C\text{-}J}$ = 24.5 GPa (@ 1.72 g cm^{-3})[53]

<table>
<tr><td>Critical diameter [cm]</td><td>1.27–1.43 mm (@ 1.52 g cm^{-3})[18], 36.5 mm (NQ-h, HBD NQ after pressing to 90% TMD, ρ = 1.61 g cm^{-3}, LASL)[36], 13.2 mm (NQ-l, HBD NQ after pressing to 90% TMD, ρ = 1.61 g cm^{-3}, LASL)[36], 36.5/38.1 mm (@ 1.62 g cm^{-3}, 91.0% TMD, pressed NQ)[52], d_c = 50 mm (NQ-h @ 70% TMD)[52], d_c = 36 mm (NQ-h @ 80% TMD)[52], d_c = 36 mm (NQ-h @ 90% TMD)[52]

critical diameter for detonation, d_c (mm)[66]:

<table>
<tr><td rowspan="2">Material</td><td colspan="7">% TMD</td></tr>
<tr><td>70</td><td>75</td><td>80</td><td>85</td><td>90</td><td>93</td><td>98</td></tr>
<tr><td>NQ-h (~100 µm)</td><td>49</td><td>41.5</td><td>36.5</td><td>35</td><td>36.5</td><td>> 37</td><td>> 37</td></tr>
</table>
</td></tr>
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<table>
<tr><td></td><td>The LBD NQ failure diameter as a function of charge density[19]:
<table><tr><th rowspan="2">charge density (g/cm³)</th><th colspan="2">charge diameter (mm)</th></tr><tr><th>detonates</th><th>fails</th></tr><tr><td>1.0</td><td>25.4</td><td>–</td></tr><tr><td>1.21</td><td>15.9</td><td>14.3</td></tr><tr><td>1.52</td><td>14.3</td><td>12.7</td></tr></table></td></tr>
<tr><td>Critical T [°C]</td><td>200–204 (exptl.)[55, 60], 204[55, 60], 198 (T_m)[19]</td></tr>
<tr><td>Trauzl test [cm³, % TNT]</td><td>101% TNT[10, 13], 78–101% TNT[18, 35], 302[78]</td></tr>
<tr><td>Sand test [g]</td><td>36.0 g (200 g bomb)[10, 13], 81–84% TNT[35], 73.5–84% TNT[18], 36.0 g sand crushed (cf. 48.0 g by TNT) corresponds to 73.5% TNT[28]</td></tr>
<tr><td>Ballistic mortar test</td><td>104% TNT[10, 13, 18, 28, 35, 84]</td></tr>
<tr><td>Lead block</td><td>7 mm shortening (40 g NQ exploded on 67 mm diameter Pb block)[50]</td></tr>
<tr><td>Lead block compression test</td><td>73% TNT[18]</td></tr>
<tr><td>Koenen [mm/type]</td><td><1/C (bottom of tube split)[57]</td></tr>
<tr><td>Initiation efficiency</td><td>0.20 g LA or 0.10 g tetryl are required for initiation[18], sensitivity to initiation varies with crystal size[18], large quantities detonated by blasting cap containing 1.5 g MF[18], 0.20 g LA minimum detonating charge[72], 0.20 g LA minimum detonating charge[13], 0.10 g tetryl minimum detonating charge[13], NQ completely detonates using detonator containing 1.5 g fulminate[50], can only be exploded with a detonator[82]</td></tr>
<tr><td>Gap test</td><td>gap test results obtained with two different donors[42]:
<table><tr><th rowspan="2">Material</th><th colspan="6">50% values</th></tr><tr><th>Donor</th><th>Gap (mm)</th><th>Shock velocity, U (mm/s)</th><th>ΔU (%)</th><th>P_u' (kbar)</th><th>ΔP_u' (%)</th></tr><tr><td>NQ (@ 1.59 g/cc)</td><td>Tetryl pellets (@ 1.51 g/cc)</td><td>11.7</td><td>4.185</td><td></td><td>83.7</td><td></td></tr><tr><td rowspan="2">NQ (@ 1.59 g/cc)</td><td rowspan="2">Pentolite 50–50 pellets (@ 1.56 g/cc)</td><td>13.5</td><td>4.955</td><td></td><td>92.5</td><td></td></tr><tr><td></td><td>4.885</td><td>± 1.4</td><td></td><td>± 5</td></tr></table>G_{50} = 5.00 mm (NQ @ 1.609 g cm^{-3}, 90.4% TMD)[56], NQ-I, ρ_0 = 0.90 g/cc, 50.3% TMD, 50% pressure (P_g) = 22.9 kbar (extrapolated)[76]</td></tr>
</table>

LSGT [cm]

G_{50} = 5.00 mm, L_{95} = 0.5 mm (@ 1.609 g cm^{-3})[19], LSGT^2 = 5.0 mm (NQ-h, HBD NQ after pressing to 90% TMD, ρ = 1.61 g cm^{-3}, LASL)[36], LSGT^2 = 5.0 mm (NQ-l, HBD NQ after pressing to 90% TMD, ρ = 1.61 g cm^{-3}, LASL)[36], 0 mm (NOL)[45], 8 mm (LANL)[45], P_{50} = 9.07 GPa (@ 1.64 g cm^{-3}, NOL-LSGT)[57], NQ-l, ρ_0 = 0.90 g/cc, 50.3% TMD, 50% pressure (P_g) = 21.2 kbar[76]

Gap test results for NQ, LANL LSGT[18]:

Density (g/cm^3)	% voids	Sensitivity (mm)
1.715 (pressed)	3.5	No explosions
1.609 (pressed)	9.6	5.00

L_g = 20 in. × 10^2 (@ 1.609 g cm^{-3}, 90.4% TMD, pressed NQ, LASL LSGT)[52], L_g = 47 in. × 10^2 (@ 1.61 g cm^{-3}, 90.6% TMD, pressed NQ, NSWC LSGT)[52]

NQ/NaCl (90/10) @ 93.8% TMD requires 100 kbar initiation pressure (6 mm) (cardboard cylinder with 42.5 mm inner diameter, LSGT cylinder with 36 mm inner diameter, 42 mm outer diameter, 140 mm length, 2 mm air gap to witness plate, RDX + 4% wax donor charge with diameter 42 mm and height 2 × 21 mm, attenuator of PMMA disks of 42 mm diameter and 1.5 mm thickness)[68]

50% gap, all charges isostatically pressed, [b] indicates HBD, [c] indicates LBD[75]:

TMD (g cm^{-3})	Exptl. ρ (g cm^{-3})	% TMD	Gap (cards)
1.78	1.61[b]	90.6	47
	1.63 [c]	91.4	35
	1.64[b]	92.1	32
	1.64[b]	92.1	36

NQ/NaCl (90/10), TMD = 1.81 g cm^{-3}, exptl. ρ = 1.70 g cm^{-3}, 93.8% TMD, gap = 27 cards[75]

LBD = low-bulk density, HBD = high-bulk density, I = isostatic press, H = hydraulic press, P = packed by hand, regular test, all charges are conditioned and fired at 25 °C[76]:

Material	Density		50% point		Particle size	Comments
	g/cc	% TMD	Cards	kbar		
NQ-L (NQ, LBD)	0.56P	31.2	216 ± 1	17		Crystals needle-like and frequently hollow, LBD = low-bulk density
	0.90P	50.6	194	21		
	1.20I	67.4	121	48		
	1.40I	78.5	84	61		
	1.51I	85.0	60	73		
	1.63I	91.4	35	90		
NQ	1.39I	78.0	109	52	Fine	Ground, 50–60% 10 micron
NQ	1.44I	81.0	98	56	Fine	
NQ	1.50I	84.5	81	63	Fine	
NQ-H (NQ, HBD)	1.35 H	75.9	140	(41)	51	HBD = high-bulk density
	1.44I	80.9	85	(61)	38	
	1.64I	92.1	36	(89)	51	
NQ-H	1.16P	65.1	196	21	64	
NQ-H	1.33 H	74.7	128	46	64	
NQ-H	1.40I	78.9	90–95	58	64	
NQ-H	1.51I	85.1	68	69	64	
NQ-H	1.61I	90.6	47	81	64	
NQ-H	1.64I	92.1	32	93	64	
NQ-H	1.39I	78.0	98	56	95	
NQ-H	1.44I	80.7	80	63	95	
NQ-H	1.44I	80.8	79	64	95	
NQ-H	1.52I	85.4	68	69	95	
NQ-H	1.33I	74.9	128	46	100	
NQ-H	1.39 H	77.9	100	55	100	
NQ-H	1.44I	80.7	86	60	100	
NQ-H	1.42I	79.7	94	59	100	Pentolite booster
NQ/NaCl, 90/10	1.701	93.6	27 ± 2	99	95/na	DLT went at 25 cards

SSGT [cm]

LANL SSGT[18]:

Density (g/cm^3)	% voids	Sensitivity (mm)
1.575 (pressed)	11.8	No explosions

NQ, TMD = 1.78 g/cm^3, (1) = no mixed response zone[74]:

Loading pressure (kpsi)	Density (g/cm^3)		% TMD	Sensitivity (DBG)			
	AVG.	s		AVG.	g	s_m	*N*
1.3	0.954	0.0105	53.6	6.387	0.0458	0.0244	28
2.	1.021	0.0095	57.4	6.951	0.1016	0.0500	28
4.1	1.161	0.0098	65.2	8.285	0.1379	0.0685	22
8.	1.273	0.0062	71.5	9.689	–	–	28 (1)

5 s explosion *T* [°C]
5 s ignition *T* [°C]
Ignition *T* [°C]
Detonating *T* [°C]

275[13, 18], 275 (dec., cook-off)[72]

275 (US value), 270 (Russian value) (dec.)[34]
185[47], does not ignite[57]
275[61], 275 (5 s)[10]

Thermal stability

Weight loss of NQ (%) @ different *T* (glass tubes without glass stoppers, heating using Al block thermostats) NQ needle-type crystals, 3.8–4.0 µm grain size, bulk $\rho = 0.3$ g cm^{-3} (% mass loss/no. of days)[27]:
@ 132 °C; 1.1/1, 1.2/6, 1.3/15, 1.4/22, 1.4/28[27]
@ 145 °C; 1.9/1, 2.9/6, 6.3/15, 8.9/22, 10.9/28[27]
@ 160 °C; 9.3/1, 20.1/6, 22.6/15, 23.4/22, 24.7/28[27]
@ 190 °C; 39.9/1, 48.0/6, 56.9/15, 63.0/22, 63.3/28[27]

weight loss of NQ (%) @ different *T* (glass tubes without glass stoppers, heating using Al block thermostats) NQ rhombohedral particles, <50 µm grain size (50%), bulk $\rho = 0.8$–1.1 g cm^{-3} (% mass loss/no. of days)[27]:
@ 132 °C; 1.6/1, 11.0/6, 21.5/15, 22.5/22, 27.7/28[27]
@ 145 °C; 2.3/1, 25.0/6, 26.8/15, 27.1/22, 27.3/28[27]
@ 160 °C; 27.2/1, 30.7/6, 31.8/15, 32.0/22, 32.5/28[27]
@ 190 °C; 40.2/1, 48.0/6, 57.7/15, 64.0/22, 64.3/28[27]

Weight loss of NQ (%) @ different *T* (glass tubes with glass stoppers, heating using Al block thermostats) NQ needle-type crystals, 3.8–4.0 µm grain size, bulk $\rho = 0.3$ g cm^{-3} (% mass loss/no. of days)[27]:
@ 132 °C; 1.7/1, 1.8/6, 2.0/15, 2.0/22[27]
@ 145 °C; 2.3/1, 4.6/6, 9.3/15, 12.3/22[27]
@ 160 °C; 28.1/1, 32.7/6, 33.8/15, 34.3/22[27]
@ 175 °C; 42.4/1, 46.9/6, 50.7/15, 53.9/22[27]
@ 190 °C; 60.0/1, 60.5/6, 61.4/15, 61.6/22[27]

<table>
<tr><td></td><td>Weight loss of NQ (%) @ different T (glass tubes with glass stoppers, heating using Al block thermostats) spherical NQ, 200–500 µm grain size (50%), bulk ρ = ~ 1.0 g cm^{-3} (% mass loss/no. of days)[27]:
@ 132 °C; 1.6/1, 54.1/6, 68.0/15, 68.2/22[27]
@ 145 °C; 2.1/1, 63.7/6, 63.4/15, 63.4/22[27]
@ 160 °C; 2.5/1, 50.4/6, 50.6/15, 50.9/22[27]
@ 175 °C; 48.0/1, 50.7/6, 53.7/15, 57.3/22[27]
@ 190 °C; 61.1/1, 62.5/6, 62.5/15, 62.6/22[27]

Thermal stability is not impaired by moisture[61]

Weight losses of NQ, when its solns. are heated in an autoclave at 120 °C for 48 h (in %)[71]:

<table><tr><td>In acid medium (pH = 3.9–6)</td><td>0.19</td></tr><tr><td>In neutral medium (pH = 7–9)</td><td>0.51</td></tr><tr><td>In alkaline medium (pH = 8–9)</td><td>2.74</td></tr></table></td></tr>
<tr><td>100 °C heat test [% mass loss]</td><td>0.18% mass loss in first 48 h[13], 0.09% mass loss in second 48 h[13], no explosions in 100 h[13]
0.48% mass loss in first 48 h, 0.09% mass loss in second 48 h, no explosions in 100 h[18, 28]</td></tr>
<tr><td>LLNL reactivity test</td><td>0.02–0.05 cm^3 gas evolved per 0.25 g sample[18, 30]</td></tr>
<tr><td>International heat test @ 75 °C</td><td>0.04% mass lost in 48 h[13, 18, 28]</td></tr>
<tr><td>Vacuum stability test [cm^3/h]</td><td>0.37 cc/40 h @ 100 °C[13], 0.44 cc/40 h @ 120 °C[13, 72], 0.1 mL/5 g @ 120 °C, 40 h[21], 0.37 cc gas evolved by 1 g in 48 h[28], similar stability to TNT @ 120 °C[18], 0.0–0.1 mL/g gas evolved after 48 h @ 120 °C[19], similar stability with that of TNT[18]

Data from[19]

<table><tr><td>Test</td><td>Results</td></tr><tr><td>Vacuum</td><td>Gas evolved after 48 h @ 120 °C (mL/g)</td></tr><tr><td>NQ per MIL-N-494A</td><td>0.0–1.0</td></tr><tr><td>Water recryst. HBD NQ</td><td>1.4–3.6</td></tr><tr><td>DMF recryst. HBD NQ</td><td>0.6–1.2</td></tr></table></td></tr>
<tr><td>Vapor pressure [atm @ °C]</td><td>1.43 × 10^{-11} mm Hg @ 25 °C[49, 59, 67]</td></tr>
<tr><td>Volatility</td><td>None[13, 28]</td></tr>
</table>

Solubility [g/mL]

Solubility, g/100 g (%) in[13]:

Solvent	°C	%
Water	25	0.44
	100	9.0
1.0 M KOH	25	1.2
40% sulfuric acid	0	3.4*
	25	8.0*

* g/100 cc soln.

0.42–0.44 g/100 mL H_2O @ 25 °C[18], 8.25 g/100 mL H_2O @ 100 °C[18], both forms (α-NQ and β-NQ) are slightly soluble in EtOH and nearly insoluble in Et_2O[18]

Solubility of NQ in sulfuric acid[18]:

Sulfuric acid % in water	*T* (°C)	g dissolved per 100 cc
0	0	0.12
	25	0.42
15	0	0.3
	25	0.55
20	0	0.45
	25	1.05
25	0	0.75
	25	1.8
30	0	1.3
	25	2.9
35	0	2.0
	25	5.2
40	0	3.4
	25	8.0
45	0	5.8
	25	10.9

g NQ dissolved in 100 g solvent[19]:

Solvent	20 °C	40 °C	60 °C
Water	0.36	0.75	1.6
DMSO	24	25	28
DMF	14	–	20
MeOH	0.3	0.6	–
Methyl ethyl ketone	0.13	0.20	–
Butyl acetate	0.07	0.08	0.1
n-Octane	0.003	0.008	–

H_2O solubility @ 25 °C: 3,200 mg/L[43], 4.4 g/L H_2O @ 25 °C[50], 82.5 g/L H_2O @ 100 °C[50], aqueous solubility = 4,200 mg/L @ 25 °C[59], slightly soluble in cold water and EtOH[61], moderately soluble in hot water[61], 2.6 g/L in H_2O @ 25 °C (*Haag*)[63, 64], 4.4 g/L in H_2O @ 25 °C (*van der Schalie*)[63], 4,400 mg/L H_2O @ 25 °C[67]

Saturated solns. of NQ in sulfuric acid[50]:

Conc. of H_2SO_4 solvent (%)	Solubility of NQ (g/100 cc)	
	@ 0 °C	@ 25 °C
45	5.8	10.9
40	3.4	8.0
35	2.0	5.2
30	1.3	2.9
25	0.75	1.8
20	0.45	1.05
15	0.30	0.55
0	0.12	0.42

Solubility in binary solvent mixtures @ 25 °C (g/100 g of solvent) after 5 min stirring[69]:

Solvent	NQ
DMSO	33
NMP	21
DMSO 20.8%	24
NMP 79.2% DMF	15
DMF 71.7% DMSO 28.3%	21

Solubility of NQ in DMF (g/100 g DMF) after 5 min stirring: 15 @ 25 °C[69], 20 @ 60 °C[69], 28 @ 98 °C[69]

β-NQ is more soluble than α-NQ in water @ 25–100 °C but @ T<25 °C the α-form is more soluble than the β-form and @ T>100 °C the α-form is more soluble than the β-form[71]

Solubility of NQ (g) in 100 g solvent @ 20 °C[71]:

Solvent	Solubility (g)
Ether	0.04
Ethyl alcohol	0.18
Acetone	0.19
Methyl alcohol	0.50
Pyridine	1.75
Water	0.27
Water	1.18 @ 50 °c
Water	10.36 @ 100 °C

Solubility of NQ (g) @ 20 °C in 100 g acid[71]:

HNO_3 conc.	Solubility (g)
5	0.6
10	1.6
20	3.0
50	5.8
87	22.3

Solubility of NQ (g) in 100 cc sulfuric acid[71]:

H_2SO_4 conc.	NQ Solubility	
	0 °C	25 °C
45	5.8	10.9
40	3.4	8.0
35	2.0	5.2
30	1.3	2.9
25	0.7	1.8
20	0.4	1.0
15	0.3	0.5

<table>
<tr><td></td><td>4.4 g dissolves in 1 L H_2O @ 25 °C (α-NQ)[82], 82.5 g dissolves in 1 L H_2O @ 100 °C (α-NQ)[82], slightly soluble in EtOH and MeOH (<0.5%, α-NQ)[82], practically insoluble in Et_2O (α-NQ)[82], soluble in conc. acids (α-form)[82], soluble in cold alkaline solns. (with dec., α-NQ)[82]

Solubility in dil. sulfuric acid, values @ 0 °C and 25 °C calcd. from lit. data[87]:

<table>
<tr><td rowspan="2">% H_2SO_4</td><td colspan="3">g NQ/100 g acid soln.</td></tr>
<tr><td>0 °C</td><td>13 °C</td><td>25 °C</td></tr>
<tr><td>5.8</td><td></td><td>0.37</td><td></td></tr>
<tr><td>17.0</td><td>0.399</td><td></td><td>0.623</td></tr>
<tr><td>17.2</td><td></td><td>0.65</td><td></td></tr>
<tr><td>20.0</td><td></td><td>0.72</td><td></td></tr>
<tr><td>20.9</td><td>0.577</td><td></td><td>1.113</td></tr>
<tr><td>24.8</td><td>0.640</td><td></td><td>1.525</td></tr>
<tr><td>28.2</td><td></td><td>1.37</td><td></td></tr>
<tr><td>29.8</td><td>1.235</td><td></td><td>2.225</td></tr>
<tr><td>44.7</td><td>5.134</td><td></td><td>8.250</td></tr>
</table>

Solubility in water in range 30–70 °C: log (solubility in g/100 g water) = –1,963.2/T + 6.1255[87], solubility in water >70 °C: log (solubility in g/100 g water) = –2,167.0/T + 6.7215 however hydrolytic autocatalysis occurs[87], 0.050 g/100 mL ethyl acetate @ 19 °C[87], 0.267 g/100 mL acetone @ 19 °C[87], 0.166 g/100 mL 96% EtOH @ 19 °C[87], 0.302 g/100 mL MeOH @ 19 °C[87], 1.750 g/100 mL pyridine @ 19 °C[87], insoluble in benzene, $CHCl_3$, CCl_4 and toluene[87]</td></tr>
<tr><td>Batch sorption</td><td>K_{ow} = 0.172 ± 0.012[43], K_d (sandy soil) = <0.02 L/kg[43], K_d (clayed, organic-rich soil) = 0.38 ± 0.04 L/kg[43]</td></tr>
<tr><td>Hygroscopicity</td><td>None @ 30 °C with 90% RH[13], essentially nonhygroscopic[18, 61], nonhygroscopic[10]</td></tr>
<tr><td>Photosensitivity</td><td>Undergoes photodegradation readily[59], aqueous solns. of NQ more readily photolyzed than aqueous RDX solns. with UV irradiation (254 nm)[59], photodegradation by sunlight of NQ in natural water similar to that of RDX[59]</td></tr>
<tr><td>Compatibility</td><td>Dec. in excess of 45% sulfuric acid[13], chemically reactive but lit. indicates little or no reaction with metals[61], partial hydrolysis in hot water[71], intensive dec. in boiling water[71]</td></tr>
</table>

<table>
<tr><td></td><td>Weight loss (%) of NQ when its sons. are heated in an autoclave at 120 °C for 48 h[71]:

<table><tr><td>Soln.</td><td>NQ weight loss (%)</td></tr><tr><td>Acid medium (ph 3.9–6)</td><td>0.19</td></tr><tr><td>Neutral medium (ph 7–9)</td><td>0.51</td></tr><tr><td>Alkaline medium (pH 8–9)</td><td>2.74</td></tr></table></td></tr>
<tr><td>$\Delta H^{o}_{sublimation}$ [kJ/mol]</td><td>139.7 ± 2.3[54], 142.7 (exptl.)[58], 102.9 (calcd., QSPR)[58]</td></tr>
<tr><td>Heat capacity, C_p [J g^{-1} K^{-1}]</td><td>C_p^{298} = 30.9 cal mol^{-1} K^{-1}[79]

Data from[19]

<table><tr><td>Material</td><td>Heat capacity @ constant pressure (cal/g-°C)</td><td>T range (°C)</td></tr><tr><td>LBD NQ[a]</td><td>0.242 + 0.0011 T(°C)</td><td>37 < T < 167</td></tr><tr><td>HBD NQ[b]</td><td>0.269 + 0.00007 T(°C)</td><td>37 < T < 167</td></tr></table>
[a] Low-bulk density, in accordance with material specification MIL-N-494A, [b] high-bulk density NQ recryst. from water, median particle diameter ~ 300 µm</td></tr>
<tr><td>Thermal conductivity, κ [W m^{-1} K^{-1}]</td><td>LBD NQ = low-bulk density NQ, data from[19]

<table><tr><td>Material</td><td>Density (g/cm^3)</td><td>Conductivity (cal/cm-s-°C)</td><td>T range (°C)</td></tr><tr><td rowspan="2">LBD NQ</td><td>1.65</td><td>10.1 × 10^{-4}</td><td>25 < T < 50</td></tr><tr><td>1.69</td><td>9.8 × 10^{-4}</td><td>25 < T < 50</td></tr></table></td></tr>
<tr><td>Diffusion coefficient [cm^2/s]</td><td>0.102 (air)[59], 1.04 × 10^{-5} (water)[59]</td></tr>
<tr><td>Log K_{ow}</td><td>–0.83[59], –0.89 @ 25 °C[63, 67], 0.148 @ 25 °C[63], –0.89–0.156[64]</td></tr>
<tr><td>Log K_{oc}</td><td>–0.356[59], 1.3[64]</td></tr>
<tr><td>Biodegradation</td><td>NQ is not biotransformed aerobically[59], partial conversion to nitrosoguandine occurs on prolonged anaerobic treatment with activated sewage sludge containing nutrients[59], NQ not biodegradable in soils unless high levels of glucose present[59]</td></tr>
<tr><td>pK_a</td><td>12.8 (est.)[64]</td></tr>
<tr><td>pH</td><td>5.5 (saturated aqueous soln. @ 25 °C)[18]</td></tr>
<tr><td>Rifle bullet test</td><td>100% unaffected (5 trials)[13, 18]</td></tr>
</table>

<table>
<tr><td>Plate dent test</td><td>Brisance = 95% TNT, $\rho = 1.50$ g cm^{-3}, not confined, pressed, method A[13], 95% TNT[18]

Data from[19]:

<table>
<tr><th>Charge diameter (mm)</th><th>Density (g/cm^3)</th><th>Dent depth (mm)</th><th>Charge height (mm)</th></tr>
<tr><td>12.7</td><td>0.25</td><td>0.56</td><td>76.2</td></tr>
<tr><td>12.7</td><td>0.40</td><td>0.79</td><td>76.2</td></tr>
</table></td></tr>
<tr><td>Booster sensitivity test</td><td>Condition = pressed, tetryl = 100 g, wax inches for 50% detonation = 0.67, $\rho = 1.41$ g cm^{-3}[13, 72]</td></tr>
<tr><td>Combustion performance</td><td>Theoretical combustion performance of neat NQ as calculated with NASA CEA code[68]:

<table>
<tr><th>Unit</th><th>0.1 MPa</th><th>1 MPa</th><th>10 MPa</th><th>100 MPa</th></tr>
<tr><td>Temperature, K</td><td>1,836</td><td>1,837</td><td>1,838</td><td>1,849</td></tr>
<tr><td>ɣ</td><td>1.2674</td><td>1.2693</td><td>1.2698</td><td>1.2642</td></tr>
<tr><td>MW, g mol^{-1}</td><td>20.811</td><td>20.813</td><td>20.819</td><td>20.924</td></tr>
<tr><td>CO, mol%</td><td>16.883</td><td>16.886</td><td>16.886</td><td>16.746</td></tr>
<tr><td>CO_2, mol%</td><td>3.115</td><td>3.113</td><td>3.115</td><td>3.174</td></tr>
<tr><td>H_2, mol%</td><td>23.101</td><td>23.106</td><td>23.082</td><td>22.486</td></tr>
<tr><td>H_2O, mol%</td><td>16.886</td><td>16.886</td><td>16.886</td><td>17.112</td></tr>
<tr><td>N_2, mol%</td><td>39.995</td><td>39.998</td><td>39.999</td><td>40.115</td></tr>
</table></td></tr>
<tr><td>Fugacity</td><td>290–300 cc[71]</td></tr>
<tr><td>Brisance</td><td>16.5 mm[71]</td></tr>
<tr><td>Dust explosion</td><td>≥4.1 kg/m^3[83]</td></tr>
<tr><td>Wedge test</td><td>[a]NQ mean particle diameter = 300 µm, cubic crystals; [b]NQ as long needle crystals, needle diameter = few µm[19]:

<table>
<tr><th>Density (g/cm^3)</th><th>Distance, x*, and time, t*, to detonation (mm and µs)</th><th>Pressure range (GPa)</th></tr>
<tr><td>1.659–1.723[a]</td><td>$\log P = (1.44 \pm 0.07) - (0.15 \pm 0.08) \log x^*$
$\log P = (1.32 \pm 0.03) - (0.15 \pm 0.07) \log t^*$</td><td>$13.35 < P < 26.28$</td></tr>
<tr><td>1.688[b]</td><td>$\log P = (1.51 \pm 0.02) - (0.26 \pm 0.03) \log x^*$</td><td>$21.2 < P < 27.1$</td></tr>
</table></td></tr>
</table>

Manometric bomb

T = 1,990 °C (@ 0.20 g cm^{-3}, manometric bomb, 139 cc volume, $T_{expl.}$ based on pressure measured)[50], 907 °C (manometric bomb expts., NQ agglomerated under 3,600 kg/cm^2, broken up into grains of 2–3 mm diameter, fired in bomb of 22 cc capacity, *Patart's* value, considered to be too low)† [50], >1,773 °C (0.20 mm diameter Pt wire in bomb was melted by explosion)[50]

Patart's exptl. results from manometric bomb expts.† [50]:

Loading ρ (g cm^{-3})	Pressure (kg/cm^2)
0.15	1304, 1584, 1416 } 1435
0.20	2060, 2122 } 2091
0.25	3092, 3068 } 3080
0.30	4118, 4038 } 4078

† calcd. from this data: covolume = 1.60, force = 7,140, T of explosion = 907 °C (considered too low by *Patart*)[50]; if NQ is compressed too strongly, incomplete dec. can occur, 3,600 kg/cm^2 pressure is too high (*Muraour* and *Aunis*)[50]

NQ compressed under 650 kg/cm^2, fired in manometric bomb, 22 cc vol., @ 0.20 g cm^{-3}, primer = 1 g black powder gave pressure = 1,737 kg/cm^2[50]

NQ compressed under 1,000 kg/cm^2, fired in manometric bomb, 22 cc vol., @ 0.20 g cm^{-3}, primer = 1 g black powder gave pressure = 1,975 kg/cm^2[50]

Calcd. values based on exptl. data[50]: $T_{expl.}$ = 2,098 °C, covolume = 1.077, force = 9,660, pressure = 2,463 kg/cm^2 (@ 0.20 g cm^{-3})[50]

Radiation sensitivity

Vacuum stability test data from[86]:

Exposure rate (R/h)	Total dose (R)	100 °C cc/g/40 h	120 °C cc/g/40 h	200 °C cc/2 g/2 h
8 × 10^5	Control		0.47	11 + (15 min)
	1.3 × 10^7		0.49	11 + (10 min)
	1.1 × 10^8		0.71	11 + (12 min)
	1.0 × 10^9	12.15	11 + (30 mins)	

DTA for irradiated NGu @ 20 °C/min[86]:

Total dose (R)	Endotherms		Exotherms	
	Onset (°C)	Peak (°C)	Onset (°C)	Peak (°C)
0	230	240	240	249
1.3×10^7	230	237	237	246
1.1×10^8	233	235	235	241
1.05×10^9	229	229	229	237
1.44×10^9	225	226	226	234

TGA for irradiated NGu[86]:

Total dose (R)	Heating rate (°C/min)	Weight (mg)	Start of dec. (°C)	10% weight loss temp. (°C)	Total weight loss (%)	Remarks
0	20	7.7	205	248	14 @ 249 °C	Deflagrated @ 249 °C
1.3×10^7	20	8.45	203	245	17 @ 249 °C	Deflagrated @ 249 °C
1.1×10^8	20	8.0	185	231	22 @ 244 °C	Deflagrated @ 244 °C

Effect of gamma radiation on the mpt. and color[86]:

Total dose (R)	mpt. (°C)	Color
0	239	White
1.3×10^7	237	Off-white
1.1×10^8	232	Yellowish white
1.0×10^9		White

IS for irradiated explosives, 50% fire height in inches, Bruceton method (P.A. apparatus, 2 kg mass)[86]:

Total Co^{60} gamma dose (R)	$\bar{X}$ mean (in)	σ std. dev. (in)
0	27.78	2.22
1.3×10^7	20.70	2.21
1.1×10^8	24.83	1.49
1.0×10^9	36 +	

Effect of gamma radiation on explosion T (5 s explosion T in °C) and activation energy (kcal/mol)[86]:

Total dose (R)	5 s explosion T (°C)	Apparent activation energy (kcal/mol)
0	288	17.91
1.3×10^7	282	14.72
1.1×10^8	285	15.04

Effect of gamma radiation on rates of detonation[86]:

Total dose (R)	Density (g/cc)	Density after irradiation (g/cc)	Rate of detonation (m/s)	Detonation pressure (kbar)
0	1.54	–	7,485	216
1.3×10^7	–	156	Would not detonate	
1.1×10^8	Pellets crumbled			

Refractive indices	Light λ = 5,893 Å, @ 25 °C: $\alpha = 1.526 \pm 0.002$, $\beta = 1.694 \pm 0.002$, $\gamma = 1.81 \pm 0.01$[87]

Propagation characteristics of NQ/H_2O mixtures, data from[83]:

Mixture composition, wt. %		Propagation test results Pipe diameter (in)				
NQ	H_2O	1.27 ½	3.81 $1^1/_2$	5.08 2	6.35 $2^1/_2$	7.62 cm 3 in
80	20	Y				Y
70	30	N		N		Y
60	40			N		
40	60			N		

Y = yes, N = no incomplete

†	**NQ**[5, 30]	**NQ**[18, 23]	**NQ**[24]	**NQ**[25]	**NQ**[26]	**NQ**[19]	**NQ**[87]
Chemical formula	$CH_4N_4O_2$	$CH_4N_4O_2$	$CH_4N_4O_2$	$CH_4N_4O_2$	$CH_4N_4O_2$	$CH_4N_4O_2$	$CH_4N_4O_2$
Molecular weight [g mol^{-1}]	104.07	104.07	104.07	104.07	104.07	104.07	104.07
Crystal system	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic
Space group	*F d d* 2 (no. 42)	*F d d* 2 (no. 42)	*F d d* 2 (no. 42)	*F d d* 2 (no. 42)	*F d d* 2 (no. 42)		
a [Å]	17.6181(14)	17.58(9)	17.6152(5)	17.6390(5)	17.64(3)	17.58	17.47
b [Å]	24.848(2)	24.82(12)	24.8502(7)	24.8730(7)	24.883(4)	24.84	24.50
c [Å]	3.5901(4)	3.58(2)	3.5880(1)	3.5903(1)	3.5950(5)	3.58	3.59
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]	1,571.7(3)	1,562.08	1,570.62	1,575.19	1,578.2(4)		
Z	16	16	16	16	16	16	16
ρ_{calc} [g cm^{-3}]	1.759(2)	1.77004	1.76	1.755	1.752		1.78
T [K]	293	295	295	295	293		

† Previous literature reported >1 polymorph, current literature reports only one crystal structure (orthorhombic) but that crystals can have two habits[27]

≥2 crystalline forms exist: α-NG and β-NG[18] and the two forms can be separated by fractional crystallization from water[18]:

α-NG[18]	**β-NG[18]**
Precipitated on addition of H_2O to soln. of NG dissolved in conc. sulfuric acid	Cryst. from hot water
Long, thin, lustrous flat needles	Fern-like clusters of small, thin, elongated plates
Form most commonly used in explosives	
Obtained by reaction of guanidine with nitric acid followed by dehydration	Obtained by nitration of guanidinium sulfate and $(NH_4)_2SO_4$ which results from hydrolysis of dicyanamide
α-NG and *β*-NG have the same mpt.	
α-NG and *β*-NG have similar chemical and physical properties	
α-NG and *β*-NG vary in solubilities	
Refractive index: α-NG = 1.52, β-NG = 1.694, γ-NG = 1.81.	

Properties of crystalline NG: colorless, hollow needles with length:diameter ratio of ~10 with LBD on crystallization from aqueous nitrating solution[57], improved bulk density (HBD) on work-up. Colorless, spherical crystals with high-bulk density SHBD on recrystallization from ethylene glycol, DMF or DMSO[57]

Property	LBD	HBD	SHBD
Max. bulk ρ (g cm^{-3})	0.3	0.9	1.15
Crystal ρ (g cm^{-3})	1.71–1.73	1.75	1.76
Particle morphology	Fine/hollow needles	Plates, bundles	Spherical grains
Particle dimensions (μm)	Length: 30–70 Width: 3–6	Diameter: 60	Diameter: 250
Specific surface area (m^2 g^{-1})	20–25	3–4	<0.5
Predominant uses	Triple-base propellants	Rocket propellants	High explosives

Crystals of β-NQ which are crystallized from water are plate shaped[71], if these β-NQ crystals are dissolved in sulfuric acid and the soln. is decanted into water then crystals of α-NQ are obtained[71]

α-NG and β-NG cryst. forms are both orthorhombic, elongated rod crystals with axial ratios *a*:*b*:*c* of 0.708:1:0.144; cleavage occurs parallel to *c*-axis; 16 molecules per unit cell[87]

NQ crystallizes in slender needles which mat into a felt-like mass[87]

NQ crystallized from dilute acetic acid produces crystals in which 70–80% have hollow cavities, only 10–20% of crystals are hollow aggregates when crystallized from water[87]. Fine crystals obtained by spraying saturated aqueous NQ soln. into a countercurrent of dry air, or by adding saturated aqueous NQ soln. to cold water[87].

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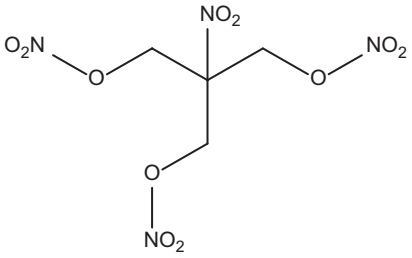
Nitroisobutylglycerol trinitrate

Name [German, acronym]: [2-Nitro-3-(nitrooxy)-2-[(nitrooxy)methyl]propyl] nitrate, nitroisobutyl-glycerintrinitrate, nitroisobutylglycerine trinitrate, nitroisobutanetriol trinitrate, NIB-glycerine trinitrate [Nitroisobutylglycerintrinitrat, NIBTN, NIBGT, NIBGTN]

Main (potential) use: Explosive, gelatinizing agent for nitrocellulose[7], in gelignite[18], suitable for low temperature applications especially in the production of liquid explosives[18], plastic explosives, powder explosives, gun propellants and rocket propellants[18]

Structural formula:



	NIBTN
Formula	$C_4H_6N_4O_{11}$
Molecular mass [g mol^{-1}]	286.11
Appearance at RT	Liquid with low volatility and no odor @ RT[5], oily liquid[12], yellow oil, more viscous than NG[13], slightly yellowish, viscous, syrupy, odorless but burning to taste liquid[15], pale yellow viscous oily liquid[18], industrial product dark yellow[18], colorless or light yellow oily transparent liquid (NIBTN specification)[18]
IS [J]	2 Nm[7], 4.9 (25 cm, 2 kg mass, 20 mg sample, B.M.)[3], 15–25 cm (2 kg mass)[5], 6 cm (2 kg mass)[8, 13], 25 cm (2 kg mass)[8], similar to that of NG[12], 15 cm (2 kg hammer, lower explosion limit)[18], 25 cm (2 kg hammer, 100% explosion)[18]
FS [N]	Friction pendulum test = 6% (cf. 16% for NG)[18]
N [%]	19.58
$\Omega(CO_2)$ [%]	±0

<table>
<tr><td>$T_{glass\ transition}$ [°C]</td><td>Highly viscous @ 0 °C and like the melted glass can be drawn into a wire[18], hard wax like solid @ freezing point[18], hard wax below freezing point[5]</td></tr>
<tr><td>$T_{m.p.}$ [°C]</td><td>−35, −39[3, 18], −39 (freezing point)[5], <−35 (freezing point)[15], −39 (freezes)[3, 12], −35 (freezes)[5, 13, 18]</td></tr>
<tr><td>$T_{dec.}$ [°C]</td><td>179.9 (onset), 200.6 (peak max), 217.8 (end T) (DSC @ 10.0 K/min, pinhole cover)[14], 179.9 (exo, onset), 200.6 (exo, peak max) (DSC 10 K/min)[19]

Nonisothermal TG data[19]:

<table>
<tr><th rowspan="2">β/K min^{-1}</th><th rowspan="2">T_{ot}</th><th rowspan="2">T_i</th><th colspan="2">mass loss/%</th><th rowspan="2">L_{max}/% min^{-1}</th><th rowspan="2">T_p/°C</th><th rowspan="2">T_{oe}/°C</th></tr>
<tr><th>Stage 1</th><th>Residue/%</th></tr>
<tr><td>7.0</td><td>163.4</td><td>124.7</td><td>99.78</td><td>0.03</td><td>−22.43</td><td>183.7</td><td>200.8</td></tr>
<tr><td>10.0</td><td>171.0</td><td>126.9</td><td>99.86</td><td>0.06</td><td>−36.47</td><td>187.5</td><td>212.3</td></tr>
<tr><td>15.0</td><td>180.9</td><td>129.3</td><td>96.71</td><td>1.07</td><td>−66.64</td><td>194.2</td><td>215.2</td></tr>
<tr><td>20.0</td><td>184.7</td><td>132.2</td><td>96.96</td><td>1.20</td><td>−90.34</td><td>197.6</td><td>223.2</td></tr>
</table>
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</td></tr>
<tr><td>ρ [g cm^{-3}]</td><td>1.735[1], 1.6171 (@ 20 °C)[5, 18], 1.68[7, 8], 1.64 (@ 20 °C)[3, 8, 9], sp. gr. = 1.68[12], 1.68 (@ RT)[13], sp. gr. = 1.68 (@ 15°)[15]</td></tr>
<tr><td>Heat of formation</td><td>50.0 kcal/mol (Q_f^V)[9], 168.7 kcal/kg[15], 200.83 kJ/mol (@ constant volume)[5, 18], 226.35 kJ/mol (@ constant pressure)[5, 18]</td></tr>
<tr><td>Heat of combustion</td><td>2,217.52 kJ/mol (@ constant volume)[5], 530.5 kcal/mol (Q_c^V)[9], 1,856 kcal/kg (@ C^V)[15], heat of comb. = 2,217.51 kJ/mol (@ constant volume)[18], heat of comb. = 7,765.5 J/g (@ constant volume)[18], 2,205.2 kJ/mol (ΔH_c, heat of comb.)[19]</td></tr>
<tr><td></td><td></td></tr>
<tr><td></td><td>Calcd. (EXPLO5 6.03)</td><td>Lit. values</td><td>Exptl.</td></tr>
<tr><td>$-\Delta_{ex}U^o$ [kJ kg^{-1}]</td><td>6,897</td><td>1,707 kcal/kg (explosive dec.)[12, 15]

7.15 MJ/kg (heat of explosion)[16]

6,924 [H_2O (g)][18]

7,389 [H_2O (l)][18]</td><td>6,924 [H_2O (g)][5]

7,389 [H_2O (l)][5]

7,755[6]

7,661 [H_2O (l)][7]

7,226 [H_2O (g)][7]</td></tr>
</table>

T_{ex} [K]	4,634	4,870 °C[18]	4,870 °C[5]
$p_{C\text{-}J}$ [kbar]	309		
VoD [m s^{-1}]	8,604 (@ 1.68 g cm^{-3})	7,780 (@ 1.64 g cm^{-3} (TMD), calcd., R-P method)[11] 8,820 (@ 1.800 g cm^{-3}, calcd., K-J)[14]	7,600 (@ 1.68 g cm^{-3})[7] 7,860 (@ 1.64 g cm^{-3})[2, 5, 13] 1,000–1,500 (@ 1.64 g/cc, glass tube, 10 mm diameter, 1 mm wall thickness)[8]* 7,860 (@ 1.64 g/cc, glass tube, 10 mm diameter, 1 mm wall thickness)[8]* 7,860 (@ 1.60 g cm^{-3})[9] 7,860 (@ 1.64 g cm^{-3}, liq., 0.39 in charge diameter, confined in glass, 1 mm wall)[3]
V_0 [L kg^{-1}]	7,670	705[18]	705[4, 5, 7] 801[6]

* The VoD values are reported to be of high (7,860 m/s) or low (1,000 m/s) order depending on the method of initiation[8]

Trauzl test [cm^3, % TNT]	55% TNT[8], 195–110% NG[12], 540[17]
Sand test [g]	28 g (200 g bomb, 0.2 g sample absorbed by 0.2 Kieselguhr)[3], 56 g sand crushed (cf. 52 g for NG)[9]

<table>
<tr><td>Brisance compression heights</td><td>Caste brisance meter, galvanized steel sample container, 1 mm wall thickness, 40 g sample, no. 8 tetryl detonator as initiator, copper cylinder 10 × 15 mm without precompaction[5, 18]:

<table><tr><th>Compression height of Cu cylinder (mm)</th><th>Relative pressure (kg/cm^2)</th></tr><tr><td>12.07</td><td>2,493</td></tr><tr><td>11.97</td><td>2,552</td></tr><tr><td>12.64</td><td>2,156</td></tr><tr><td>12.55</td><td>2,210</td></tr></table></td></tr>
<tr><td>5 s explosion T [°C]
5 s ignition T [°C]
Initiation T [°C]</td><td>180–185 (dec./deflagration)[8], 255[18]
185[3, 10], 255[5]
180[12]</td></tr>
<tr><td>Thermal stability</td><td>Nonisothermal TG data, β = °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.[14]:

<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>7.0</td><td>163.4</td><td>183.7</td><td>200.8</td><td>158.5</td></tr><tr><td>10.0</td><td>171.0</td><td>187.5</td><td>212.3</td><td></td></tr><tr><td>15.0</td><td>180.9</td><td>194.2</td><td>215.2</td><td></td></tr><tr><td>20.0</td><td>184.7</td><td>197.6</td><td>223.2</td><td></td></tr></table>
Less thermally stable than NG and slow dec. on storage[5, 18], critical T for thermal dec. = 158.5 °C[19]</td></tr>
<tr><td>Vapor pressure [atm @ °C]</td><td>Lower than that of NG[18]

Vapor pressures @ different T[5, 18]:

<table><tr><th>T (°C)</th><th>40</th><th>50</th><th>60</th><th>70</th><th>80</th></tr><tr><td>Vapor pressure (mm Hg)</td><td>2.74 × 10^{-4}</td><td>5.00 × 10^{-4}</td><td>14.8 × 10^{-4}</td><td>33.6 × 10^{-4}</td><td>79.3 × 10^{-4}</td></tr></table></td></tr>
<tr><td>Volatility</td><td>0.127 × 10^{-3} g mg/cm^2/24 h mass loss @ 25 °C[3, 8], less volatile than NG[5, 13, 18], slightly volatile @ RT[18], highly volatile @ 50 °C[18], 0.127 × 10 mg/cm/24 h @ 25 °C[18], little volatility @ RT and slightly volatile @ 30 °C, volatile @ 50 °C[5], 0.127 × 10 mg/cm/day @ 25 °C[5]</td></tr>
</table>

<table>
<tr><td></td><td>Volatilization losses (%) @ different T, approx. values from graph[18]:
<table>
<tr><td rowspan="2">Time (h)</td><td colspan="3">T (°C)</td></tr>
<tr><td>68</td><td>70</td><td>80</td></tr>
<tr><td>2</td><td>0.02</td><td>0.03</td><td>0.1</td></tr>
<tr><td>4</td><td>0.03</td><td>0.5</td><td>0.15</td></tr>
<tr><td>6</td><td>0.04</td><td>0.07</td><td>0.25</td></tr>
<tr><td>8</td><td>0.05</td><td>0.1</td><td>0.3</td></tr>
<tr><td>10</td><td>0.06</td><td>0.13</td><td>0.4</td></tr>
<tr><td>12</td><td>0.07</td><td>0.15</td><td>0.5</td></tr>
<tr><td>14</td><td>0.08</td><td>0.16</td><td>0.55</td></tr>
<tr><td>16</td><td>0.09</td><td>0.17</td><td>0.65</td></tr>
<tr><td>18</td><td>0.1</td><td>0.19</td><td>0.75</td></tr>
</table></td></tr>
<tr><td>Viscosity [cP]</td><td>308.55 @ 20 °C[5, 18], 8–9 times that of NG[18], highly viscous @ 0 °C[5]</td></tr>
<tr><td>Solubility [g/mL]</td><td>Soluble in MeOH, EtOH, acetone, Et_2O, ethylene dichloride, $CHCl_3$ and benzene[3], insoluble in water, CS_2 and petroleum ether[3], 0.081% in water @ 20 °C[5, 18], soluble in Et_2O, acetone, benzene, CCl_4, CH_2Cl_2, nitrobenzene and nitrotoluene as well as nitroaromatics[5], very soluble in Et_2O, acetone[13], soluble in EtOH, benzene, $CHCl_3$[13], insoluble in ligroin[13], immiscible with H_2O[12], soluble in most common organic solvents except petroleum ether[12], miscible with many organic solvents, for example, Et_2O, acetone, benzene, ethyl acetate, CCl_4, CH_2Cl_2, nitrobenzene, nitromethane[18]</td></tr>
<tr><td>Compatibility</td><td>Hydrolyzed in dilute basic solns., hydrolyzation constant = 1.81×10^{-3}[5], thermal dec. catalyzed by acids, bases, water and other impurities[5]</td></tr>
<tr><td>$\Delta H_{dec.}$ [J/g]</td><td>569.8 (heat release)[14], 153.4 kJ/mol (ΔH_d, heat of dec.)[19]</td></tr>
<tr><td>Refractive index</td><td>$n^{D}_{25} = 1.4896$[3, 5, 18], $n^{D}_{30} = 1.4874$[3]</td></tr>
<tr><td>82.2 °C KI test</td><td>Minutes[3]</td></tr>
<tr><td>Surface tension [dyne/cm]</td><td>Data from[18]:
<table>
<tr><td>T (°C)</td><td>20</td><td>30</td><td>40</td><td>50</td><td>60</td></tr>
<tr><td>Surface tension (dyne/cm)</td><td>56.62</td><td>55.87</td><td>55.13</td><td>54.38</td><td>53.64</td></tr>
</table></td></tr>
<tr><td>Abel test</td><td>>25 min @ 72 °C (NIBTN specification)[18]</td></tr>
</table>

[1] Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© **1994–2017** ACD/Labs).
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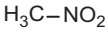
Nitromethane

Name [German, acronym]: Nitromethane, nitrocarbol [nitromethan, NM]
Main (potential) use: Component of binary explosives, synthetic intermediate for synthesis of explosives, propellants, solvent, rocket fuel component[42], fuel in binary high explosives[48], liquid rocket fuel[48]

Structural formula:



	NM
Formula	CH_3NO_2
Molecular mass [g mol^{-1}]	61.04
Appearance at RT	Very pale yellow colored liquid, colorless liquid[42], colorless liquid with fruity odor[48], oily liquid with moderately strong, disagreeable odor[49]
IS [J]	>40, 40[7], >78.5 (12 tool)[8], 100 cm[15], 640 mm (drop height, Rotter impact test)[35], 361 mm (drop height, Rotter impact test + 5% DETA)[35], 89 cm (median height, Rotter apparatus)[45], dropping 10 kg weight from 25 cm results in 0–8% explosions[42], $<^1/_{10}$ tests positive (25.0 cm drop height, 3.63 kg mass, B.M. apparatus)[52]
FS [N]	>360
N [%]	22.95
Ω(CO_2) [%]	−39.32
$T_{m.p.}$ [°C]	−28[1], −29[8, 14, 49], −28.55[15], −29 (freezing point)[42] Pressure dependence of the melting point (approx. values)[34]: 300 °C/0.4 GPa, 322 °C/0.46 GPa, 330 °C/0.48 GPa, 362 °C/0.8 GPa, 380 °C/1.0 GPa, 420 °C/1.38 GPa[34]
$T_{b.p.}$ [°C]	101.2[42], 101[42], 100[48], bp_{760} = 101.2[49], bpt_{100} = 46.6[49], bp_{40} = 27.5[49], bp_{20} = 14.1[49], bp_{10} = 2.8[49], bp_5 = −7.9[49], $bp_{1.0}$ = −29[49], 101[50]
T_{dec} [°C]	>300 (DSC)[7], dec. occurs >1.54 GPa and 433 K[34], 3,418 K (Adiabatic dec. *T*)[37]
ρ [g cm^{-3}]	1.131 (@ 298 K)[2], 1.13130 (@ 298 K)[3], 1.313 (@ 298 K, TMD)[8], 1.13 (@ TMD, liquid)[38], sp. gr. = 1.132 (@ 15 °C)[42], 1.14[48], $d^{25}{}_4$ = 1.1322[49], 1 gallon weighs 9.5 lb[49],

	sp. gr. data from[42]:

Temperature (°C)	ρ (g/cm^3)	Ostwald viscosity
10	1.1490	0.748
25	1.1287	0.625
40	1.1080	0.533

Heat of formation	−113 ± 0.4 kJ/mol ($\Delta_f H°$ (liquid), exptl., NIST database)[51], −113.1 ± 0.63 kJ/mol ($\Delta_f H°$ (liquid), exptl., NIST database)[51], −89.04 ± 0.75 kJ/mol ($\Delta_f H°$ (liquid), exptl., NIST database)[51], −112.97 kJ mol^{-1} (standard heat of form.)[13], −21.8 kcal/mol[15], − 1,853 kJ/kg (ICT thermochemical database)[4], −1,850.75 J/g (standard heat of form.)[13], −27.0 kcal/mol[9], −1,853.5 kJ/kg[5], −19.3 kcal/mol ($\Delta H_f°$ (g))[33], −28.5 kcal/mol ($\Delta H_f°$)[33], −27.0 kcal/mol (ΔH_f)[32], 318.3 kcal/kg[41], −27.6 ± 0.2 kcal/mol ($\Delta_f H°$ (c))[25], −17.8 kcal/mol ($\Delta_f H°$ (g))[25], −27.0 kcal/mol ($\Delta_f H°$)[26], −113.1 kJ/mol[38], −113 kJ/mol (enthalpy of form.)[48], −17.4 kcal/mol (ΔH_f(g)°, calcd., ccCA-P)[53], −18.8 kcal/mol (ΔH_f(g)°, calcd., ccCA-S3)[53], −18.1 kcal/mol (ΔH_f(g)°, calcd., ccCA-PS3)[53], −17.7 kcal/mol (ΔH_f(g)°, calcd., G3)[53], −16.0 kcal/mol (ΔH_f(g)°, calcd., G3(MP2))[53], −17.8 ± 0.2 kcal/mol (ΔH_f(g)°, exptl.)[53]
Heat of combustion	ΔH_c = −1,69.5 ± 0.2 kcal/mol (liq.)[25, 33], heat of comb. = −11.63 kJ/g (exptl.)[37], heat of comb. = 2,881 kcal/kg (@ C^V)[41], heat of comb. = 175.25 kcal/mol (@ 25 °C)[15], $\Delta_c H°$ (liquid) = −709.6 ± 0.4 kJ/mol[51], $\Delta_c H°$ (liquid) = −703 ± 1 kJ/mol[51], $\Delta_c H°$ (liquid) = −709.15 ± 0.59 kJ/mol[51], $\Delta_c H°$ (liquid) = −733.25 ± 0.75 kJ/mol[51], $\Delta_c H°$ (liquid) = −709.2 kJ/mol[51]

	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]	4,593	162 kcal/g [H_2O (l)][14] 136 kcal/g [H_2O (g)][14] 4,566 (calcd., ICT code)[4] 5.1 GPa (detonation energy)[31] 5.29 MJ/kg (calcd., SD method)[43] 4.54 MJ/kg (heat of explosion)[44] 4,300 [H_2O (g)][48]	3,975 [H_2O (g)][12] 4,539.6 J/g[13] 123 kcal/g [H_2O (l)][14] 106 kcal/g [H_2O (g)][14] 1.23 kcal/g (highly confined samples in calorimeter) [H_2O (l)][17] 1.23 kcal/g [H_2O (l)][18] 5,137 J/g (@ 1.13 g cm^{-3}, heavily confined charge) [H_2O (l)][28]

			4,482 J/g [H_2O (g)] (@ 1.13 g cm^{-3}, heavily confined charge)[28] 4,381 J/g (@ 1.130 g cm^{-3}, det. energy, cylinder test)[28] 4.59 GPa (detonation energy calcd. from cylinder test data)[31]
T_{ex} [K]	3,126	2,960 (@ 1.128 g cm^{-3})[16] 3,311 (@ 1.14 g cm^{-3}, calcd.)[26] 3,121 (@ 1.52439 g cm^{-3}, calcd., THOR, C (g))[27] 3,417 (@ 1.470588 g cm^{-3}, calcd., THOR)[27] 3,430 (@ 1.515152 g cm^{-3}, calcd., Monte Carlo simulation with carbon)[27] 3,274 (@ 1.531395 g cm^{-3}, calcd., Monte Carlo simulation)[27] 3,513 (@ 1.531394 g cm^{-3}, calcd., thermchemical)[27] 3,043 (calcd., ICT code)[4] 3,456 (@ 1.13 g cm^{-3}, calcd., $\Delta H_f = -27.0$ kcal/mol, KLRR/C, THEOSTAR-T)[32] 3,451 (@ 1.13 g cm^{-3}, calcd., $\Delta H_f = -27.0$ kcal/mol, BKWC, THEOSTAR-T)[32]	3,430[9, 27] 3,380 (@ 1.128 g cm^{-3})[16] 3,700[17] 3,380[17, 27] 3,400 (@ 1.13 g cm^{-3})[32]

		3,138 (@ 1.13 g cm^{-3}, calcd., ΔH_f = −27.0 kcal/mol, BKWR, THEOSTAR-T)[32] 3,376 (calcd., SD method)[43] 3,220 (@ 1.13 g cm^{-3}, calcd. BKWR)[9] 3,580 (@ 1.13 g cm^{-3}, calcd. BKWS)[9]	
$p_{C\text{-}J}$ [kbar]	130	58 (@ 1.16 g cm^{-3} (TMD), calcd., R-P method)[20] 132 (@ 1.13 g cm^{-3}, calcd., BKW)[21] 141 (@ 1.135 g cm^{-3}, calcd., Xiong)[22] 133 (@ 1.125 g cm^{-3}, calcd., K-J)[23] 137 (@ 1.14 g cm^{-3}, calcd., K-J)[23] 142 (@ 1.159 g cm^{-3}, calcd., K-J)[23] 151 (@ 1.128 g cm^{-3}, calcd.)[16] 141 (@ 1.14 g cm^{-3}, calcd.)[26] 115 (@ 1.52439 g cm^{-3}, calcd., THOR, C(g))[27] 108 (@ 1.470588 g cm^{-3}, calcd., THOR)[27] 118 (@ 1.515152 g cm^{-3}, calcd., Monte Carlo simulation with carbon)[27]	125[8, 9, 27] 135 [11] 13 GPa[13] 141 (@ 1.16 g cm^{-3})[17] 130[14, 18] 138[20] 133[24] 0.125 MPa[14] 144 (@ 1.135 g cm^{-3})[22] 140 (@ 1.125 g cm^{-3})[23] 133 (@ 1.14 g cm^{-3})[23] 148 (@ 1.159 g cm^{-3})[23] 129 (@ 1.128 g cm^{-3})[16] 129 (@ 1.14 g cm^{-3})[16] 130 (@ 1.128 g cm^{-3})[16] 120[27] 141[27]

		121 (@ 1.531395 g cm^{-3}, calcd., Monte Carlo simulation)[27] 123 (@ 1.531394 g cm^{-3}, calcd., Thermochemical)[27] 139.7 MPa (calcd., ICT code)[4] 12.6 GPa (@ 1.13 g cm^{-3}, calcd., $\Delta H_f = -27.0$ kcal/mol, KLRR/C, THEOSTAR-T)[32] 12.1 GPa (@ 1.13 g cm^{-3}, calcd., $\Delta H_f = -27.0$ kcal/mol, BKWC, THEOSTAR-T)[32] 13.5 GPa (@ 1.13 g cm^{-3}, calcd., $\Delta H_f = -27.0$ kcal/mol, BKWR, THEOSTAR-T)[32] 134 (@ 1.13 g cm^{-3}, calcd. BKWR)[9] 130 (@ 1.13 g cm^{-3}, calcd. BKWS)[9]	12 GPa (@ 1.130 g cm^{-3}, heavily confined charge)[28] 12.5 GPa (@ 1.128 g cm^{-3}, cylinder test)[31] 12.5 GPa (@ 1.13 g cm^{-3})[32] 12.0 GPa (@ 1.130 g cm^{-3})[39]
VoD [m s^{-1}]	6,500 (@ TMD)	5,510 (@ 1.16 g cm^{-3} (TMD), calcd., R-P method)[20] 6,910 (@ 1.16 g cm^{-3} (TMD), calcd., *Aizenshtadt*)[20] 6,480 (@ 1.16 g cm^{-3} (TMD), calcd., K-J)[20] 6,500 (@ 1.13 g cm^{-3}, calcd., BKW)[21] 6,412 (@ 1.135 g cm^{-3}, calcd., *Xiong*)[22] 6,871 (@ 1.128 g cm^{-3}, calcd.)[16] 6,480 (@ TMD, calcd., K-J)[24]	6,350 (@ 1.13 g cm^{-3})[6, 8, 9] 6,300 (@ 1.14 g cm^{-3})[11, 16] 6,320 (@ 1.13 g cm^{-3})[13] 6,210 (glass tube, $^1/_{32}$ in diameter, no ρ given)[15] 6,280 (Fe tube, no ρ given)[15] 6,060 (Brass tube, no ρ given)[15] 20,000 feet/s (stainless steel tube, $^1/_2$ in diameter, no ρ given)[15] 6,370 (@ 1.16 g cm^{-3})[17]

		6,370 (@ 1.14 g cm^{-3}, calcd.)[26] 6,325 (@ 1.52439 g cm^{-3}, calcd., THOR, C(g))[27] 5,918 (@ 1.470588 g cm^{-3}, calcd., THOR)[27] 6,438 (@ 1.515152 g cm^{-3}, calcd., Monte Carlo simulation with carbon)[27] 6,641 (@ 1.531395 g cm^{-3}, calcd., Monte Carlo simulation)[27] 6,493 (@ 1.531394 g cm^{-3}, calcd., Thermochemical)[27] 6,350 (@ 1.13 g cm^{-3}, calcd., $\Delta H_f = -27.0$ kcal/mol, KLRR/C, THEOSTAR-T)[32] 6,280 (@ 1.13 g cm^{-3}, calcd., $\Delta H_f = -27.0$ kcal/mol, BKWC, THEOSTAR-T)[32] 6,670 (@ 1.13 g cm^{-3}, calcd., $\Delta H_f = -27.0$ kcal/mol, BKWR, THEOSTAR-T)[32] 6,560 (@ 1.13 g cm^{-3}, calcd. BKWR)[9] 6,590 (@ 1.13 g cm^{-3}, calcd. BKWS)[9]	6,290 (@ 1.14 g cm^{-3})[19] 6,200 (@ 1.13 g cm^{-3}, aquarium test detonation, 2.5 cm, Teflon)[21] 6,320 (@ 1.135 g cm^{-3})[22] 6,280 (@ 1.128 g cm^{-3})[14] 6,290 (@ 1.128 g cm^{-3})[16] 6,320 (@ TMD)[24] 6,300 (@ 1.13 g cm^{-3})[15] 6,300 (@ 1.14 g cm^{-3})[26] 6,280 (@ 1.130 g cm^{-3}, heavily confined charge)[28] 6,287 (@ 1.128 g cm^{-3}, cylinder test)[31] 6,350 (@ 1.13 g cm^{-3})[32] 6,280 (@ 1.130 g cm^{-3})[39] 6,352 (@ 1.14 g cm^{-3}, D_i) (D_i = ideal detonation velocity)[43] 6,067 (@ 1.14 g cm^{-3}, D_f) (D_f = detonation velocity for critical detonation diameter)[43] 6,290 (@ 1.138 g cm^{-3}, confined)[48]
V_0 [L kg^{-1}]	1,004		1,059[10] 1,092 mL/g[13]

Copper cylinder wall velocity data, wall thickness/diameter ratio = 0.1, all cylinders were 305 mm long, PETN with $\rho = 1.763$ g cm^{-3} is the reference explosive[38]:

Initial ρ (g/cm^3)	Inner diameter (mm)	Wall thickness (mm)	Wall velocity, mm/μs @ 25.4 mm diameter for $r-r_0$ equal to			Velocity-squared cf. with PETN for the same configuration, 5 comparison $r-r_0$ equal to		
			6 mm	12.5 mm	19 mm	6 mm	12.5 mm	19 mm
1.13	50.83	5.199	1.045	1.180	1.230	−55.1	−52.1	−52.8

Summary of code calculations with measured detonation velocities and detonation energies derived from JWL's[38]:

Initial ρ,(g/cm^3)	PETN-adjusted BKWR Tiger, LLNL library $\theta = 1{,}850$ K (v)			JCZ3, LLNL library (v)			CHEQ V2.4 (v)		
	2.2	4.1	6.5	2.2	4.1	6.5	2.2	4.1	6.5
1.13	7	4	7	0	−4	−2	−8	−9	−7

Derivation of the total energy of detonation, E_0 from the measured heat of detonation (the final state is assumed to be at 1 atmosphere for all gaseous products, including water, @ 298 K. Code calculated energies with the 1,800 K freeze are also included)[38]:

Measured ρ (g/cm^3)	Measured confined heat of detonation (kJ/cm^3)	Density from ref.[38]	Heat of detonation, density from ref.[38]	Energy of detonation, E_0 (kj/cm^3)			
				From heat of detonation	Freeze @ 1,800 K		
					Tiger BKWR	Tiger JCZ3	CHEQ
1.13	−5.80	1.13	−5.80	−5.2	−5.7	−5.3	−5.4

Comparison of measured "CJ" temperatures using optical pyrometry[38]:

Exptl. ρ (g/cm^3)	Max. measured t (k)	Calculated CJ temp K			Wavelength (μm)
		Tiger BKWR	Tiger JCZ3	CHEQ	
1.13	3,300–3,500	3,000	3,400	3,800	0.6–0.9

<table>
<tr><td>Critical diameter [cm]</td><td>25 mm (for detonation propagation in Fe tubes)[15], 7 mm (for detonation propagation in Brass tubes)[15]

measurements of d_c and initiation pressure, P_i[36]:
<table><tr><td>Material</td><td>Form</td><td>ρ_0, g/cc</td><td>P_i, kbar</td><td>d_c, mm</td></tr><tr><td>NM</td><td>liq., 20 °C</td><td>1.13</td><td>82</td><td>18</td></tr></table>
2.8 mm (bronze tubes, 3.18 mm wall thickness)[43], 13.5 mm (glass shell)[43], 6.3 mm (0.08 mm thin Cu foil inserted into 13.5 mm glass shell)[43]</td></tr>
<tr><td>Trauzl test [cm^3, % TNT]</td><td>110–127% TNT[15], 470 cc (fugacity)[42], 345 cm^3[46], 400 cm^3[46], 430 mL/10 g[47]</td></tr>
<tr><td>Sand test [g]</td><td>8.1 g sand crushed per 1 g NM[15]</td></tr>
<tr><td>Ballistic mortar test</td><td>134% TNT[15]</td></tr>
<tr><td>Gap test</td><td>Scale I (detonator = standard commercial no. 8 Briska type, donor = 2 × 20 g pellets of tetryl pressed to ρ = 1.5 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) critical card value = 3[40]
Scale III (donor = 2 × 20 g pellets of tetryl pressed to ρ = 1.5 g/mL, each 1.5 in in diameter, gap = 4 in square cards, charge case = 3 in length of 1 ½ 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) critical card value = 24[40]

UN gap test: apparent ρ = 1,130 kg/m^3, fragmentation length = 0 cm, witness plate = no damage, result = negative[52]</td></tr>
<tr><td>5 s explosion T [°C]</td><td>430[15]</td></tr>
<tr><td>Thermal stability</td><td>Half-life of 30 d @ 250 °C[15], slow dec. @ 350 °C[15], unexpected detonation possible >300 °C[15]</td></tr>
<tr><td>Vapor pressure [atm @ °C]</td><td>37 mm Hg @ 25 °C[14]</td></tr>
<tr><td>Enthalpy of vaporization [kcal mol^{-1}]</td><td>9.2 ± 0.1[25]</td></tr>
<tr><td>Dipole moment, μ [D]</td><td>3.46 (exptl. value)[30, 35]</td></tr>
<tr><td>Dielectric constant, ε</td><td>35.9 (exptl. value)[30]</td></tr>
</table>

Solubility [g/mL]	10.5 cc dissolve in 100 cc H_2O @ 100 °C[42], readily soluble in benzene, toluene, xylene, EtOH and acetone[42], soluble in water ~ 9% @ 20 °C[42], miscible with almost all organic liquids[42], 10% in water @ 20 °C[48], slightly soluble in water (9.5% by vol. @ 20°)[49], soluble in EtOH, Et_2O, DMF[49]
Compatibility	NM explodes @ high temperatures and high pressures in the presence of impurities in a closed vessel @ 260 °C[37], reacts with formaldehyde[42]
Heat of dec. [kJ/g]	–6.33 (max. heat of dec., calcd. CHEETAH)[37], 4.84 (heat value – heat of dec., calcd. CHEETAH)[37]
Refractive index	1.3935 @ 20 °C[42], $n^{22}{}_D = 1.38056$[49]
Viscosity	Oswald viscosity values from[42]

Temperature (°C)	ρ (g/cm^3)	Ostwald viscosity
10	1.1490	0.748
25	1.1287	0.625
40	1.1080	0.533

Heat capacity [cal/mole/°C]	2.07 @ 20 °C[42], 106.22 J/mol K (@ 308 K, C_p (liq.))[51], 108.8 J/mol K (@ 313 K, C_p (liq.))[51], 105.98 J/mol K (@ 298.15 K, C_p (liq.))[51], 100 J/mol K (@ 298 K, C_p (liq.))[51]
Hess brisance	25 mm (with an auxiliary TNT cap of 5–8 g)[42]
2” steel tube test (UN A1)	Yes[47]
Flash point [°C]	36[48], 112°F[49]
Autoignition point [°C]	418[48]
pH	Aqueous solns. acidic to litmus[49], 6.12 (0.01 M aq. soln.)[49]
Koenen test	Limiting diameter <1.0 mm, negative result[18]

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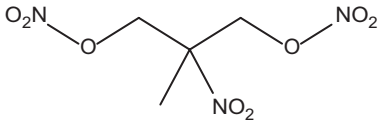
Nitromethyl propanediol dinitrate

Name [German, acronym]: 1,3-Propanediol-2-methyl-2-nitrodinitrate, 2-methyl-2-nitro-1,3-propanediol dinitrate

Main (potential) use: Partial substitute for NG[4]

Structural formula:



	Nitromethyl propanediol dinitrate		
Formula	$C_4H_7N_3O_8$		
Molecular mass [g mol^{-1}]	225.11		
Appearance at RT	Waxy crystals[4]		
IS [J]	>50, Fl = 86% rel. to PA[4], 11 cm (2 kg mass)[4], $H_{50\%}$ = 27–46 cm (Bruceton no. 5 apparatus, 2 kg mass)[4]		
FS [N]	>360		
N [%]	18.67		
$\Omega(CO_2)$ [%]	–24.9		
$T_{m.p.}$ [°C]	38[4], 37.4[4]		
$T_{b.p.}$ [°C]	Dec. @ 200 °C[4]		
$T_{dec.}$ [°C]	Ignites >240[4], dec. in 10 min @ 82.2[4], dec. @ 200 °C within 5 sec[4]		
ρ [g cm^{-3}]	1.545 (@ 293 K)[1]		
Heat of formation	–374.0 kJ/mol (enthalpy of form., exptl.)[5], –340.0 kJ/mol (enthalpy of form., calcd., emp.)[5], –379.6 kJ/mol (enthalpy of form., calcd., S-D method)[5]		
Heat of combustion	531.4 kcal/mol[3], 531.4 kcal/mol (Q^c_v)[4]		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]			5,295 [H_2O (l)][3] 4,866 [H_2O (g)][3]
T_{ex} [K]			

$p_{C\text{-}J}$ [kbar]			
VoD [m s^{-1}]			
V_0 [L kg^{-1}]		935 (calcd., BKW-EOS)[2] 973 (calcd., JCZ3-EOS)[2] 896 (calcd., ProPEP code)[2] 913 (calcd., empirical)[2]	890[2, 3]

Trauzl test [cm^3, % TNT]	~160% TNT[4]
Sand test [g]	53 g sand crushed by 0.4 g (equivalent to tetryl)[3], 53 g sand crushed cf. 478 g for TNT (110.5% TNT)[4]
Ballistic mortar test	134–138% TNT[3], ~ 135% TNT[4]
5 s explosion *T* [°C] Explosion *T* [°C]	 Ignited >240 °C[4]
100 °C heat test [% mass loss]	15–30 min in 135° heat test[4], no explosion in 300 min in 130° heat test[4]
82.2° KI test	9–30 min[4], comparable to NG[4]
Solubility [g/mL]	Slightly soluble in water[4], soluble in EtOH, acetone, Et_2O, petrol ether[4]
Power	Nearly as powerful as TNT[4]
Brisance	More brisant than tetryl[4]
Rifle bullet test	High order detonations[4]

[1] Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© **1994–2017** ACD/Labs).
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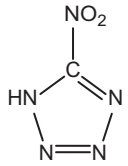
5-Nitrotetrazole

Name [German, acronym]: Nitrotetrazole, 5-nitro-1*H*-tetrazole, [nitrotetrazol, 5-Nitro-1*H*-tetrazol, HNT]

Main (potential) use: For forming corresponding salts which are promising low-toxicity, environmentally friendly, primary explosives for blasting caps and commercial primers[2]

Structural formula:



	HNT		
Formula	CHN_5O_2		
Molecular mass [g mol^{-1}]	115.05		
Appearance at RT	Colorless crystalline solid[3]		
IS [J]	$H_{100\%}$ = 25 cm (10 kg mass)[3]		
FS [N]			
ESD [J]			
N [%]	60.87		
$\Omega(CO_2)$ [%]	–6.95		
$T_{m.p.}$ [°C]	101[3]		
$T_{dec.}$ [°C]	115–120 (DTA, intensive dec. with 75% mass loss)[3]		
ρ [g cm^{-3}]			
Heat of formation	543 kcal/kg ($\Delta_f H°$)[3], 2,273 kJ/kg ($\Delta_f H°$)[2]		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]			
T_{ex} [K]			
$p_{C\text{-}J}$ [kbar]			

VoD [m s^{-1}]		8,500 (@ 1.7 g cm^{-3})[3]	~8,900 (@ 1.73 g cm^{-3})[2]
V_0 [L kg^{-1}]			
Thermal stability	Intensive dec. with 75% mass loss @ 115–120 °C (DTA)[3]		
Burn rate [mm/s]	110 @ 100 atm (FLAME database)[1]		
Hygroscopicity	Very hygroscopic[3]		
pK_a	−0.82[2, 3] (pK_{BH+} = −9.3[2])		

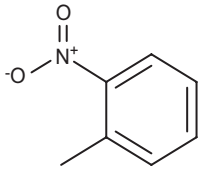
[1] R. L. Simmons, C. M. Walsh, *Designing Advanced Gun Propellants with Improved Energy Release*, ICT **2001**, Karlsruhe, Germany, pp. 43-1–43-11.
[2] M. A. Ilyushin, I. V. Tselinsky, I. V. Shugalei, *Central Eur. J. Energet. Mater.*, **2012**, *9*, 293–327.
[3] V. A. Ostrovskii, C. I. Koldobskii, *Russ. Chem. J.*, **1997**, *41*, 84.

2-Nitrotoluene

Name [German, acronym]: 1-Methyl-2-nitrobenzene, *o*-nitrotoluene [nitrotoluol, 2-MNT]

Main (potential) use: Taggant for formulations, precursor/intermediate in TNT synthesis

Structural formula:



	2-MNT	
Formula	$C_7H_7NO_2$	
Molecular mass [g mol^{-1}]	137.14	
Appearance at RT	Yellowish liquid[2]	
IS [J]	>40	
FS [N]	>360	
N [%]	10.21	
$\Omega(CO_2)$ [%]	−180.84	
$T_{m.p.}$ [°C]	−10[2], −9.55 (needles)[1], −2.9 (cryst. yellow liq.)[1]	
$T_{b.p.}$ [°C]	222[2], 221.7[1]	
ρ [g cm^{-3}]	1.629 (needles)[1], $d^{19}{}_{15} = 1.1622$[2],	
Heat of formation	2.0 kcal/mol (Q_f)[1]	
Heat of combustion	897.0 kcal/mol ($Q_c{}^v$)[1]	
	Calcd. (EXPLO5 6.03)	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]	2,717	
T_{ex} [K]	1,878	
$p_{C\text{-}J}$ [kbar]	57	
VoD [m s^{-1}]	4,649 (@ TMD)	
V_0 [L kg^{-1}]	593	

Solubility [g/mL]	Almost insoluble in water[2], soluble in EtOH, benzene, petrol ether[1, 2]
Refractive index	$n^{20}{}_{D} = 1.5472$[2], 1.5450 (needles with mpt. = –9.5 °C)[1]
Flash point [°F]	223[1]

[1] S. M. Kaye, *Encyclopedia of Explosives and Related Items*, *vol. 9*, US Army Research and Development Command, TACOM, Picatinny Arsenal, USA, **1980**.

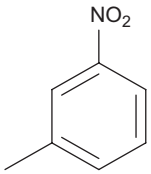
[2] *The Merck Index – An Encyclopedia of Chemicals and Drugs*, 9th edn., M. Windholz, S. Budavari, L. Y. Stroumtsos, M. N. Fertig (eds.), Merck and Co. Inc., Rahway, New Jersey, USA, **1976**.

3-Nitrotoluene

Name [German, acronym]: 3-Nitrotoluene, methylnitrobenzene, *m*-nitrotoluene [nitrotoluol, 3-MNT]

Main (potential) use: Taggant for formulations

Structural formula:



	3-MNT	
Formula	$C_7H_7NO_2$	
Molecular mass [g mol^{-1}]	137.14	
Appearance at RT	Liquid[1]	
IS [J]	>40	
FS [N]	>360	
N [%]	10.21	
Ω(CO_2) [%]	−180.84	
$T_{m.p.}$ [°C]	16, 15.5[1]	
$T_{b.p.}$ [°C]	243, bp_{760} = 231.9[1], bp_{100} = 156.9[1], bp_{40} = 130.7[1], bp_{20} = 112.8[1], bp_{10} = 96.0[1], bp_5 = 81.0[1], $bp_{1.0}$ = 50.2[1]	
ρ [g cm^{-3}]	1.157 (gas pycnometer), $d^{15}{}_4$ = 1.1630[1], $d^{20}{}_4$ = 1.1581[1], $d^{59}{}_4$ = 1.124[1], $d^{121}{}_4$ = 1.063[1]	
Heat of formation	−44 kJ/mol ($\Delta_f H°$), −233 kJ/kg ($\Delta_f U°$)	
	Calcd. (EXPLO5 6.03)	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]	2,618	
T_{ex} [K]	1,833	
$p_{C\text{-}J}$ [kbar]	55	
VoD [m s^{-1}]	4,602 (@ TMD)	
V_0 [L kg^{-1}]	591	

Solubility [g/mL]	0.498 g dissolve in 1 L H_2O @ 30 °C[1], miscible with EtOH, Et_2O[1], soluble in benzene[1]
Refractive index	$n^{30}{}_D = 1.5426$[1]

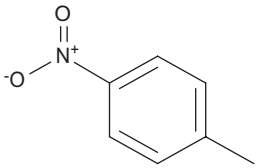
[1] *The Merck Index – An Encyclopedia of Chemicals and Drugs*, 9th edn., M. Windholz, S. Budavari, L. Y. Stroumtsos, M. N. Fertig (eds.), Merck and Co. Inc., Rahway, New Jersey, USA, **1976**.

4-Nitrotoluene

Name [German, acronym]: 4-Nitrotoluene, *p*-nitrotoluene, methylnitrobenzene [nitrotoluol, 4-MNT]

Main (potential) use: Taggant for formulations, precursor in TNT synthesis

Structural formula:



	4-MNT	
Formula	$C_7H_7NO_2$	
Molecular mass [g mol^{-1}]	137.14	
Appearance at RT	Yellow orthorhombic crystals[1], yellowish crystals[3]	
IS [J]	>40 (<100 µm)	
FS [N]	>360 (<100 µm)	
ESD [J]	>1.5 (<100 µm)	
N [%]	10.21	
$\Omega(CO_2)$ [%]	−180.84	
$T_{m.p.}$ [°C]	51, 54.5[1], 53–54[3]	
$T_{b.p.}$ [°C]	238.3[1], 234 (DSC @ 5 °C/min), 238[3]	
ρ [g cm^{-3}]	1.353 (@ 100 K), 1.1038 (@ 75/4°)[1], 1.293 (@ 298 K, gas pycnometer), 1.286[3]	
Heat of formation	10.4 kcal/mol (Q_f)[1]	
Heat of combustion	888.6 kcal/mol (Q_c^V)[1]	
	Calcd. (EXPLO5 6.03)	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]	2,618	
T_{ex} [K]	1,833	
$p_{C\text{-}J}$ [kbar]	55	
VoD [m s^{-1}]	4,602 (@ TMD)	
V_0 [L kg^{-1}]	591	

Solubility [g/mL]	Practically insoluble in water[3], soluble in EtOH, benzene, Et_2O, $CHCl_3$, acetone[1, 3]
Flash point [°C]	106[3], 223°F[1]
Refractive index	1.5382[1]

	4-Nitrotoluene[2]
Chemical formula	$C_7H_7NO_2$
Molecular weight [g mol^{-1}]	137.14
Crystal system	Orthorhombic
Space group	*Pcab* (no. 61)
a [Å]	6.43
b [Å]	14.07
c [Å]	15.66
α [°]	90
β [°]	90
γ [°]	90
V [Å^3]	1,416.76
Z	8
ρ_{calc} [g cm^{-3}]	1.286
T [K]	295

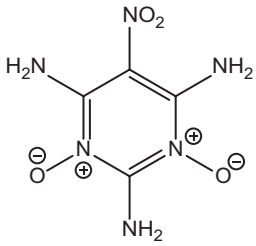
[1] S. M. Kaye, *Encyclopedia of Explosives and Related Items*, *vol. 9*, US Army Research and Development Command, TACOM, Picatinny Arsenal, USA, **1980**.
[2] J. V. Barve, L. M. Pant, *Acta Cryst.*, **1971**, *B27*, 1158–1162.
[3] *The Merck Index – An Encyclopedia of Chemicals and Drugs*, 9th edn., M. Windholz, S. Budavari, L. Y. Stroumtsos, M. N. Fertig (eds.), Merck and Co. Inc., Rahway, New Jersey, USA, **1976**.

5-Nitro-2,4,6-triaminopyrimidine-1,3-dioxide

Name [German, acronym]: 5-Nitro-2,4,6-triaminopyrimidine-1,3-dioxide, [NTAPDO, ICM-102, P6NAAA]

Main (potential) use: Future thermally stable explosive[1], promising IHE[2]

Structural formula:



	NTAPDO
Formula	$C_4H_6N_6O_4$
Molecular mass [g mol^{-1}]	202.13
Appearance at RT	Yellow solid (monohydrate)[2], orange solid (vacuum dehydration of monohydrate @ 150 °C for 5 h)[2], darker orange solid (hot recryst. of monohydrate from DMSO/EtOAc 130 °C)[2]
IS [J]	<60 (BAM)[2], H_{50} = 320 cm (2.5 kg hammer)[2]
FS [N]	>360 (BAM)[2]
ESD [J]	1.85[2]
N [%]	41.58
Ω(CO_2) [%]	−55.45
$T_{m.p.}$ [°C]	
$T_{dec.}$ [°C]	284 (DSC)[2] Onset and peak temperatures from DSC[2]:

Heating rate (°C/min)	T_e (°C)	T_p (°C)
5	264.6	280.5
10	271.9	283.7
15	274.4	286.7
0	252.5	277.1
T_{SADT}	T_b	
252.5 °C	257.7 °C	

ρ [g cm^{-3}]	1.95 (anhydrous, gas pycnometer @ 298 K)[2], 1.92 (hydrate heated @ 150 °C under vacuum for 5 h)[2]		
Heat of formation	–8.1 kJ/mol ($\Delta_f H$, calcd., isodesmic)[2]		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]			
T_{ex} [K]			
$p_{C\text{-}J}$ [kbar]		34.3 GPa (@ 1.95 g cm^{-3}, $\Delta H_f = -8.1$ kJ/mol, calcd., EXPLO5 6.02)[2]	
VoD [m s^{-1}]		9,169 (@ 1.95 g cm^{-3}, $\Delta H_f = -8.1$ kJ/mol, calcd., EXPLO5 6.02)[2]	
V_0 [L kg^{-1}]			
Critical temperature of thermal explosion, T_b [°C]	257.7 (calcd.)[2]		
Thermal stability	Heating sample from RT → 200 °C showed almost no changes in IR and Raman spectra of sample[2]		
Solubility [g/mL]	mg/100 mL solvent @ 25 °C[2]: 220 H_2O[2], 20 DMSO[2], 10 DMF[2], <8 EtOH[2], <8 MeOH[2], <8 MeCN[2], <8 acetone[2], <8 dichloromethane[2], <8 EtOAc[2]		
$T_{dehydration}$ [°C]	178 (DSC)[2]		
Self-accelerating decomposition temperature, T_{SADT} [°C]	252.5 (calcd.)[2]		

	ICM-102•H_2O[2]
Chemical formula	$C_4H_6N_6O_4$•H_2O
Molecular weight [g mol^{-1}]	220.16
Crystal system	Monoclinic
Space group	$P2_1/c$
a [Å]	10.714(2)
b [Å]	8.8863(18)

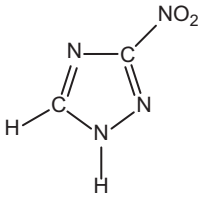
c [Å]	18.946(4)
α [°]	90
β [°]	118.50(1)
γ [°]	90
V [Å^3]	1,585.2(6)
Z	8
ρ_{calc} [g cm^{-3}]	1.845
T [K]	173

[1] S. R. Ahmad, M. Cartwright, *Laser Ignition of Energetic Materials*, John Wiley and Sons Ltd., **2015**.

[2] Y. Wang, Y. Liu, S. Song, Z. Yang, X. Qi, K. Wang, Y. Liu, Q. Zhang, Y. Tian, *Nature Comm.*, **2018**, *9*, 2444.

3-Nitrotriazole

Name [German, acronym]: 3-Nitro-1,2,4-triazole, [3-nitrotiazol]
Main (potential) use: Possible insensitive explosive candidate[3]
Structural formula:



	3-Nitro-1,2,4-triazole		
Formula	$C_2H_2N_4O_2$		
Molecular mass [g mol^{-1}]	114.08		
Appearance at RT	Yellow irregular block crystals (form I)[3], white needle crystals (form II)[3]		
IS [J]	>25 (BAM)[1], >40 (Form I, BAM)[3], >40 (Form II, BAM)[3]		
FS [N]	>36 kp (Julius-Peters)[1], 360 (Form I, BAM)[3], 360 (Form II, BAM)[3]		
ESD [J]	29.24 (Form I)[3], 29.24 (Form II)[3]		
N [%]	49.1		
$\Omega(CO_2)$ [%]	−42.08		
$T_{m.p.}$ [°C]			
$T_{phase\ transition}$ [°C]	Irreversible conversion from form II → form I >98 °C (powder X-ray diffraction)[3], form I is more stable than form II @ elevated *T*[3], forms I and II are both stable @ RT[3], form I is stable up to 200 °C whereas form II is unstable[3], 98 (exo, form II → form I, DSC @ 5 °C/min, Al crucible)[3]		
$T_{dec.}$ [°C]	217 (exo, dec. form I, DSC @ 5 °C/min, Al crucible)[3], 217 (exo, dec. form I, DSC @ 5 °C/min observed after form II undergoes exo phase transition @ 98 °C to Form I, Al crucible)[3]		
ρ [g cm^{-3}]	1.72[1], 1.72 (form I, X-ray @ 25 °C)[3], 1.79 (form II, X-ray @ 25 °C)[3]		
Heat of formation	97.9 (enthalpy of form.)[1], 146.57 kJ/mol (heat of form. $\Delta H°_f$, calcd., for form I or form II)[3]		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.

$-\Delta_{ex}U^{o}$ [kJ kg^{-1}]		4,786 (form I, calcd., EXPLO5 5.05)[3] 4,822 (form II, calcd., EXPLO5 5.05)[3]	
T_{ex} [K]		3,561 (form I, calcd., EXPLO5 5.05)[3] 3,530 (form II, calcd., EXPLO5 5.05)[3]	
$p_{C\text{-}J}$ [kbar]		24.81 GPa (form I, calcd., EXPLO5 5.05)[3] 27.45 GPa (form II, calcd., EXPLO5 5.05)[3]	
VoD [m s^{-1}]		7,947 (form I, calcd., EXPLO5 5.05)[3] 8,213 (form II, calcd., EXPLO5 5.05)[3]	
V_0 [L kg^{-1}]			
5 s explosion T [°C] Explosion T [°C]	218 (DTA/TG @ 6 °C/min)[1]		

	3-Nitrotriazole[2]	**3-Nitrotriazole (form I)**[3]	**3-Nitrotriazole (form II)**[3]
Chemical formula	$C_2H_2N_4O_2$	$C_2H_2N_4O_2$	$C_2H_2N_4O_2$
Molecular weight [g mol^{-1}]	114.08	114.08	114.08
Crystal system	Monoclinic	Tetragonal	Monoclinic
Space group	$P2_1/c$ (14)	$P4_12_12$ (92)	$P2_1/c$ (14)
a [Å]	8.7818(1)	6.8413(3)	8.7895(6)
b [Å]	10.0726(2)	6.8413(3)	10.0707(8)
c [Å]	9.9703(1)	18.8196(12)	9.9645(5)
α [°]	90	90	90
β [°]	107.081(1)	90	107.082(6)
γ [°]	90	90	90
V [Å^3]	843.03(2)	880.82(8)	843.11(10)
Z	8	8	8
ρ_{calc} [g cm^{-3}]	1.798	1.720	1.797
T [K]	100	101.8	101.8

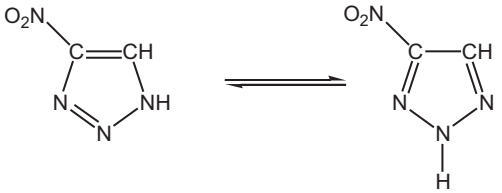
Crystallizes in two polymorphic forms: form 1 = tetragonal ($P4_12_12$) and form II = monoclinic ($P2_1/c$)[3], form II obtained on recrystallization of form I from methanol and ethyl acetate.[3]

[1] H. H. Licht, S. Braun, M. Schäfer, B. Wanders, H. Ritter, *Nitrotriazole: Chemische Struktur und Explosive Eigenschaften*, ICT **1998**, 47-1–47-15.
[2] M. Hemamalini, H.-K. Fun, *Acta Cryst.*, **2011**, *E67*, 015.
[3] P. Zhang, X. Zhao, Y. Du, M. Gozin, S. Li, S. Pang, *RSC Adv.*, **2018**, *8*, 24627–24632.

4-Nitrotriazole

Name [German, acronym]: 4-Nitrotriazole, [4-nitrotiazol]
Main (potential) use: analytical reagent

Structural formula:



	4-Nitrotriazole		
Formula	$C_2H_2N_4O_2$		
Molecular mass [g mol^{-1}]	114.06		
Appearance at RT			
IS [J]	4.5 (BAM)[1]		
FS [N]	29 kp (Julius-Peters)[1]		
N [%]	49.12		
$\Omega(CO_2)$ [%]	−42.08		
$T_{m.p.}$ [°C]			
$T_{dec.}$ [°C]			
ρ [g cm^{-3}]	1.73[1]		
Heat of formation	167.0 kJ/mol (enthalpy of form.)[1]		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]			
T_{ex} [K]			
$p_{C\text{-}J}$ [kbar]			
VoD [m s^{-1}]			

V_0 [L kg^{-1}]			
5 s explosion *T* [°C] Explosion *T* [°C]	218 (DTA/TG @ 6 °C/min)[1]		

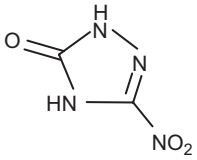
[1] H. H. Licht, S. Braun, M. Schäfer, B. Wanders, H. Ritter, *Nitrotriazole: Chemische Struktur und Explosive Eigenschaften*, ICT **1998**, 47-1–47-15.

3-Nitro-1,2,4-triazole-5-one

Name [German, acronym]: 3-Nitro-1,2,4-triazole-5-one, 5-nitro-1,2,4-triazol-3-one, 5-nitro-2,4-dihydro-3*H*-1,2,4-triazole-3-one, oxynitrotriazole, nitrotriazolone [NTO†, ONTA]

Main (potential) use: Insensitive (high) explosive, oxidizer, investigated as possible insensitive component to replace RDX in certain explosive and propellant compositions[31], nonazide inflating propellant compositions for car air bags[47] proposed for use in melt-castable, general-purpose formulations and PBXs[45, 49], melt-castable explosives (NTO-TNT mixture)[49], pressed explosives with a thermoplastic binder[49], evaluated as insensitive component to replace RDX in bomb fill[58], evaluated as ingredient to replace NaN_3 in auto air bags[58]

Structural formula:



† NTO-B corresponds to NTO which was crystallized from an NTO/H_2O/NMP/surfactant B (10/70/20/0.008) mixture; NTO-S corresponds to NTO produced in Scandinavia; NTO-W corresponds to NTO crystallized from H_2O.

	NTO
Formula	$C_2H_2N_4O_3$
Molecular mass [g mol^{-1}]	130.06
Appearance at RT	
IS [J]	>120 Nm[14], 15.85 (1st reaction)[6, 39], 71.61 (sound)[39], 7 (NTO-W, according to standard PN-EN 13,631–4, $^0/_6$ positive trials (minimum sensitivity), 5 kg mass, 0.02 g sample)[19], 6 (NTO-S, according to standard PN-EN 13631-4, $^0/_6$ positive trials (minimum sensitivity), 5 kg mass, 0.02 g sample)[19], 13 (NTO-B, according to standard PN-EN 13631-4, $^0/_6$ positive trials (minimum sensitivity), 5 kg mass, 0.02 g sample))[19], 71.61 (sound)[6], 0.6 ((no units) based on TNT = 1)[9], E_{50} = 61 J (Bruceton method, particle diameter 75–350 µm)[10], 25.6[11], 25 Nm (BAM)[15, 34], >260 cm (ERL type 12)[16], >280 cm (type 12 tool c.f. RDX= 22 cm)[18], FoI = 80–90 (3–5 mL (g) evolution, 5 kg mass, 27 mg sample (Rotter apparatus)[17], FoI = 25.3 (average powder

explosiveness, 5 kg mass, 27 mg sample (Rotter apparatus)[17], >280 cm (ERL-LASL (type 12))[17], H_{50} = 291 cm[26], 82.5 cm (20.2 J)[29], $(H_{50}Wg)^{-1}$ = >49 Nm[32], minor ignitions @ 1.3 m (glass anvil drop-weight machine, max. drop height = 1.3 m, 5 mg powder, @ 1.3 m compacted layer behaves brittle. Layer then gels compacted and compressed layers of NTO much less fragmented from lower drop heights, from 1.0 m drop-height ignition also occurs, the burning products flow around the sample @ ~ 250 ms^{-1}, sample was not completely consumed)[33], $H_{50\%}$ = 43 in (250 µm, Thiokol app.)[36], $H_{50\%}$ = 26 cm (250 µm, ABL app.)[36], H_{50} = 90 cm (5 kg hammer, E_{d50} = 45.0 J)[44], $H_{50\%}$ = 291 cm (recryst. NTO, US data)[42], $H_{50\%}$ = 75–104 cm (recryst. NTO, US data)[42], 22 (recryst. NTO, French data)[42], H_{50} = 26.2 cm (micro-NTO, WL-1 drop-weight machine, 2.5 kg mass, 35 mg sample)[47], H_{50} = 26.2 cm (nano-NTO, WL-1 drop-weight machine, 2.5 kg mass, 35 mg sample)[47], 22 (Julius-Peters apparatus)[49], Rotter FoI = 80–90 (ref. to RDX)[49], Rotter FoI = 316 (ref. to RDX)[49], >280 cm (US drop impact type 12)[49], 293 cm (US drop impact type 12B)[49], H_{50} = 50 cm (US impact sensitivity)[49], >4 m (30 kg hammer, nonreaction height)[49], >50[53], 6.6 (micro NTO)[56], 8.9 (nano NTO)[56], A_{d1} = 8%, A_{d2} = 84%, LL = 1.0 m, $A_{50\,d1}$ = 4.3 m, $A_{50\,d2}$ = 1.4[57]

Rotter FoI (mean mL of gas evolved) = 90 (3) (recryst. NTO)[42], 80 (5) (recryst. NTO)[42], 75 (6) (unrecryst. NTO)[42], 70 (6) (unrecryst. NTO)[42]

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[62]

Rotter impact data		US data	
F of I	Gas evolved (mL)	NSWC/NOL, ERL Type 12	NWC B.M. type 12
80–90	3–5	75–104	

Rotter impact data, 20 drop expts., $H_{50\%}$ = median drop height, each drop expt. has the no. of ignitions out of 20 (n_g), the fraction of ignitions (P_g), average gas volume evolved per ignition (V_g) and calcd. powder explosiveness at each level (X), $H_{50\%}$ = 128 cm, NTO sub 850 µm, data from[62]:

Drop height multiple of $H_{50\%}$	No. of fires out of 20 drops (n_g)	$P_g = n_g/20$	Average gas evolved, V_g (mL)	Explosiveness at each level, × (%)
0.67	0	0	0	0
0.75	3/40	0.075	3.1	10.6
1.0	13	0.65	2.9	10.1

	<table><tr><th>Drop height multiple of $H_{50\%}$</th><th>No. of fires out of 20 drops (n_g)</th><th>$P_g = n_g/20$</th><th>Average gas evolved, V_g (mL)</th><th>Explosiveness at each level, × (%)</th></tr><tr><td>1.5</td><td>20</td><td>1.0</td><td>7.8</td><td>27.7</td></tr><tr><td>2.0</td><td>10/10</td><td>1.0</td><td>10.0</td><td>38.2</td></tr></table> Rotter impact data, 20 drop expts., $H_{50\%}$ = median drop height, each drop expt. has the no. of ignitions out of 20 (n_g), the fraction of ignitions (P_g), average gas volume evolved per ignition (V_g) and calcd. powder explosiveness at each level (X), $H_{50\%}$ = 114 cm, NTO sub 150 µm data from[62]: <table><tr><th>Drop height multiple of $H_{50\%}$</th><th>No. of fires out of 20 drops (n_g)</th><th>$P_g = n_g/20$</th><th>Average gas evolved, V_g (mL)</th><th>Explosiveness at each level, × (%)</th></tr><tr><td>0.67</td><td>0</td><td>0</td><td>0</td><td>0</td></tr><tr><td>0.75</td><td>3/30</td><td>0.10</td><td>3.7</td><td>12.7</td></tr><tr><td>1.0</td><td>16</td><td>0.80</td><td>3.4</td><td>11.8</td></tr><tr><td>1.5</td><td>18</td><td>0.90</td><td>11.0</td><td>39.1</td></tr><tr><td>2.0</td><td>10/10</td><td>1.0</td><td>8.0</td><td>34.4</td></tr></table>
FS [N]	>353[14], >360[10, 11, 29], >360 (BAM)[17], >353 (NTO-S, Julius-Peters apparatus, $^0/_{10}$ positive trials)[19], >353 (NTO-B, Julius-Peters apparatus, $^0/_{10}$ positive trials)[19], $P_{fr.LL}$ = 400 MPa[21, 57], $P_{fr.50\%}$ = 540 MPa[21, 57], >36 kp (Julius-Peters)[34], 800 psi @ 8 ft/s (250 µm, ABL app.)[36], >353 (SNPE data, BAM)[49], >353 (South Africa data, BAM)[49], >296[53]
ESD [J]	8.9[13], spark sensitivity = 0.91 (3 mil)[18, 49], spark sensitivity = 3.40 (10 mil)[18, 49], $E_{50\%}$ = 0.47 ± 0.04 (Bruceton eqn.)[30], $E_{50\%}$ = 0.43 ± 0.05[30], $E_{50\%}$ = >8[36], >4.5 (no ignition, recryst. NTO, MRL data)[42], 0.45 (no ignition, recryst. NTO, MRL data)[42], 3.40 (recryst. NTO, US data)[42], >4.5 (no ignition, unrecryst. NTO, MRL data)[42], <4.5 (Australian data)[49], 15 (South African data)[49], >0.726 (SNPE data)[49], 8.98 (Czech data)[49]
N [%]	43.08
$\Omega(CO_2)$ [%]	−24.6
$T_{phase\ transition}$ [°C]	Crystalline NTO exists as α and β polymorphs, α-NTO is more stable[49], β-NTO recryst. from MeOH decomposed after 6 months @ RT[49], α-NTO is metastable[49]
$T_{m.p.}$ [°C]	270[14], 270–271[1], no melting point[22], 255 (dec.)[9], 260 (with dec.)[20], 543 K[49], 546 K[49], 547.9 K[49], 262[51], 270 (dec.)[53], 539.35 K[60], 547.9 K[60]
$T_{b.p.}$ [°C]	568 K[49], 568.4 K (est. T_{nbp})[60]

$T_{dec.}$ [K]

507 K (DTA @ 5 °C/min)[6, 39], 258[17], >236 (DTA)[18], NTO-B: 259.5 (onset), 262.7 (max. rate, 66% mass loss) (DSC @ 5 K/min, 3–5 mg sample, open Al_2O_3 crucibles)[19], 267 (exo peak max., DSC @ 20 °C/min)[22], 273[29], ~ 270[31], 236 (explosion, DTA/TG @ 6 °C/min)[34], 215–280 (nonisothermal TGA, pierced pan, 78% mass loss, competes with sublimation)[51], 255–270 (nonisothermal DSC @ 5 °C/min, exotherm, competes with sublimation)[51], 254 (exo, onset), 260 (exo, peak max) (DTA)[59]

TGA/DTA (10 mg sample, in air, 1 K/min, open Al pan): 179 (begin of mass loss), 219 (3% mass loss), 248 (start of exo dec.), ~ 258 (max. peak in DTA)[37]

DSC (0.3–0.5 mg sample, 10 °C/min): 264.8 (exo peak onset), 270.1 (exo peak max.)[37]

DSC (0.3–0.5 mg sample, after storing NTO @ 65.5 °C for 16 weeks, 10 °C/min): 272.5 (exo peak onset), 277.1 (exo peak max.)[37]

Dynamic DSC experiments[28]:

Heating rate (°C/min)	Mass (mg)	T_{onset} (°C)	T_{peak} (°C)	ΔH_r (J•g^{-1})
2	0.48	249.4	251.9	2,122.4
5	0.46	260.3	262.7	2,132.3
10	0.45	267.2	270.8	2,251.1
20	0.44	271.1	276.3	2,257.3

DSC experiments using interruption and rescanning method[28]:

Heating rate (°C/min)	Mass (mg)	T_{onset} (°C)	T_{peak} (°C)	ΔH_r (J•g^{-1})
10	0.40	–	267.2	2,280.0
10	0.44	254.1	263.2	1,789.5
10	0.51	256.0	257.6	1,500.9
10	0.48	257.1	250.9	1,247.9

DSC experiments (Swiss method)[28]:

Heating rate (°C/min)	Mass (mg)	E_a (kJ mol^{-1})	$\bar{E}_a$ (kJ mol^{-1})
2	0.48	314.8	
5	0.46	501.8	528.7
10	0.45	769.6	

273 (DSC @ 5 °C/min, recryst. NTO, MRL data)[42], >236 (recryst. NTO, US data)[42], 270–275 (recryst. NTO, US data)[42], 170 (onset of mass loss, nano-NTO, TG)[47], ~ 130 (onset of mass loss, micro-NTO, TG)[47]

$T_{sublimation}$ [°C]	215–280 (nonisothermal TGA, pierced pan, 78% mass loss, competes with dec., strongly heat rate dependent)[51]		
ρ [g cm^{-3}]	1.91[9, 14, 34], 1.92[2], 1.93 (crystal)[18, 53], 1.918[26], 1.93[29, 49], 1.911[49], 1.049 (bulk, particle diameter 75–350 µm)[10] NTO-S: 0.960 (loose bulk ρ)[19], 1.072 (shaken bulk ρ (5 min on sieve shaker))[19] NTO-B: 0.996 (loose bulk ρ)[19], 1.160 (shaken bulk ρ (5 min on sieve shaker))[19]		
Heat of formation	–96.7 kJ/mol[5], –14.30 kcal mol^{-1}[17], –129.4 kJ mol^{-1} (ΔH_f)[29], –97 kJ/mol (enthalpy of form.)[53], –112.3 kJ/mol [11], –24.09 kcal/mol (ΔH_f (s))[26], –130 kJ/mol (ΔH_f)[27], – 774.60 (enthalpy of form.)[14], –59.9 kJ mol^{-1} (enthalpy of form.)[34], –130.0 kJ mol^{-1} (ΔH_f)[35], –775 kJ/kg (ΔH_f, ICT thermochemical database)[38], –206.0 kcal/kg (enthalpy of form.)[40], –30.93 kcal/mol (enthalpy of form. of (s))[45, 49], –3.2 kcal/mol (enthalpy of form. of (g))[45, 49], –5.7 kcal/mol (enthalpy of form. of (g))[45, 49], –5–0.9 cal/mol (enthalpy of form. of (g))[49], –59.83 kJ/mol (enthalpy of form.)[49], –117.21 kJ/mol (enthalpy of form.)[49], –100.7 kJ/mol (enthalpy of form.)[49], –112 kJ/mol (ΔH_f)[61]		
Enthalpy of combustion [kJ/mol]	–943.4 to –995.7[49]		
	Calcd. (EXPLO5 5.04)	Lit. values	Exptl.
$-\Delta_{ex}U^{o}$ [kJ kg^{-1}]		0.982 kcal/g (Q_{max}, calcd.)[26] 3,148 (calcd., ICT code)[38]	899 kcal/kg [H_2O (g)][12] 3,148 [H_2O (l)][14] 2,993 [H_2O (g)][14]

		912 kcal/kg (@ 1.9470 g cm^{-3}, calcd.) [H_2O vapor][40] 4,100 kJ/mol (enthalpy of explosion)[49] 2,719 (@ 1.90 g cm^{-3}, calcd., LOTUSES)[61]	7,100 MJ/m^3 (E_0, @ 1.77 g cm^{-3}, det. energy based on cylinder test)[31, 41] 899 kcal/kg (@ 1.940 g cm^{-3}) [H_2O vapor][40]
T_{ex} [K]		2,288.1 (@ 1.93 g cm^{-3}, calcd. CHEETAH 6.0)[29] 2,956 (calcd., ICT code)[38] 2,389 (@1.93 g cm^{-3}, $\Delta H_f = -129.4$ kJ/mol, calcd., JAGUAR)[55] 2,700 (@ 1.90 g cm^{-3}, calcd., LOTUSES)[61]	
$p_{C\text{-}J}$ [kbar]	311[2]	349 (@ 1.93 g cm^{-3} (100% TMD), calcd., BKW)[18] 284 (@ 1.781 g cm^{-3} (92.2% TMD), calcd., BKW)[18] 316 (@ 1.853 g cm^{-3} (96% TMD), calcd., BKW)[18] 284 (@ 1.782 g cm^{-3} (92.3% TMD), calcd., BKW)[18] 316 (@ 1.855 g cm^{-3} (96.1% TMD), calcd., BKW)[18] 271 (@ 1.759 g cm^{-3} (91.1% TMD), calcd., BKW)[18]	Values from unconfined plate-dent tests[18]: 278 (@ 1.781 g cm^{-3}, 4.13 cm charge diameter)[18, 42] 260 (@ 1.853 g cm^{-3}, 4.13 cm charge diameter)[18, 42] 240 (@ 1.782 g cm^{-3}, 2.54 cm charge diameter)[18, 42] Failed (@ 1.855 g cm^{-3}, 2.54 cm charge diameter)[18, 42] 250 (@ 1.759 cm^{-3}, 1.27 cm charge diameter)[18, 42] Failed (@ 1.824 cm^{-3}, 1.27 cm charge diameter)[18, 42] 29.9 GPa (@ 1.93 g cm^{-3})[23]

<table>
<tr>
<td></td>
<td></td>
<td>300 (@ 1.918 g cm^{-3}, calcd.)[26]

33.1 GPa (@ 1.93 g cm^{-3}, calcd. CHEETAH 6.0)[29]

307 katm (@ 1.91, calcd. TIGER, BKW)[36]

106.4 MPa (calcd., ICT code)[38]

24.98 GPa (@ 1.78 g cm^{-3}, calcd., BKWC, CHEETAH 1.39)[41]

28.3 GPa (@ 1.830 g cm^{-3}, calcd., TIGER, BKWR, BKW eqn. of state)[48]

31.2 GPa (@ 1.93 g cm^{-3}, calcd., Cheetah 2.0)[53]

33.1 GPa (@ 1.93 g cm^{-3}, calcd. CHEETAH 6.0)[29]

32.7 GPa (@ 1.93 g cm^{-3}, $\Delta H_f = -129.4$ kJ/mol, calcd., JAGUAR)[55]

37.46 GPa (@ 1.90 g cm^{-3}, calcd., LOTUSES)[61]</td>
<td>Values determined using aquarium test variant[31]:

<table>
<tr><th>Property</th><th>Shot no. 1</th><th>Shot no. 2</th></tr>
<tr><td>ρ (g cm^{-3})</td><td>1.78</td><td>1.78</td></tr>
<tr><td>$P_{C\text{-}J}$ (GPa), H_2O test</td><td>24.6</td><td>24.6</td></tr>
<tr><td>$P_{C\text{-}J}$ (GPa), Calcd.</td><td>24.98</td><td>24.98</td></tr>
<tr><td>Exponent γ, H_2O test</td><td>3.40</td><td>3.40</td></tr>
<tr><td>Exponent γ, Calcd.</td><td>3.48</td><td>3.48</td></tr>
</table>

25.4 GPa (pressed @ 1.78 g cm^{-3})[31]

24.6 GPa (@ 1.78 g cm^{-3}, mod. aquarium test)[41]

24.6 GPa (est. based on cylinder test results)[48]</td>
</tr>
<tr>
<td>VoD [m s^{-1}]</td>
<td>7,860 (@ 1.80 g cm^{-3})

7,940 (@ 1.77 g cm^{-3})

8,558[2]</td>
<td>8,656 (@ TMD, calcd., CHEETAH v8.0)[24]

5,644 (@ 1.0 g cm^{-3}, calcd., BKWR)[25]

5,266 (@ 1.0 g cm^{-3}, calcd., BKWS)[25]</td>
<td>8,510 (@ 1.93 g cm^{-3})[7]

8,520 (@ 1.91 g cm^{-3})[9]

7,940 (@ 1.77 g cm^{-3})[11]</td>
</tr>
</table>

		8,070 (@ 1.918 g cm^{-3}, calcd.)[26] 8,120 (@ 1.91 g cm^{-3}, calcd. TIGER, BKW)[36] 8,000 (@ 1.78 g cm^{-3}, calcd., BKWC, CHEETAH 1.39)[41] 8,062 (@ 1.830 g cm^{-3}, calcd., TIGER, BKWR, BKW eqn. of state)[48] 8,564 (@ 1.93 g cm^{-3}, calcd., Cheetah 2.0)[53] 8,640 (@ 1.93 g cm^{-3}, $\Delta H_f = -129.4$ kJ/mol, calcd., JAGUAR)[55] 8,380 (@ 1.87 g cm^{-3}, calcd., JAGUAR)[55] 8,370 (@ 1.87 g cm^{-3}, calcd., JAGUAR)[55] 8,310 (@ 1.86 g cm^{-3}, calcd., JAGUAR)[55] 8,180 (@ 1.83 g cm^{-3}, calcd., JAGUAR)[55] 8,070 (@ 1.8 g cm^{-3}, calcd., JAGUAR)[55] 8,752 (@ 1.93 g cm^{-3}, calcd., LOTUSES)[61]	7,959 (@ 1.81 g cm^{-3})[15] 7,790 (@ 1.77 g cm^{-3})[23] 7,960 (@ 1.81 g cm^{-3})[23] 8,200 (@ 1.93 g cm^{-3})[23] 8,300 (exptl. est. LASEM method)[24] 8,535 (@ TMD, large-scale detonation test)[24] 7,740 (@ 1.83 g cm^{-3}, cylinder test, Cu tube, 25 mm internal diameter, 2.5 mm wall thickness)[48] NTO pressed @ 1.80 g cm^{-3} in cylindrical pellet form, diameter: length ratio = 1, pellet diameters = 14.5, 16.0 mm, 20 mm, 25.0 mm, 30.0 mm, charges initiated by booster of phlegmatized RDX @ 1.6 g cm^{-3} with charge diameter and length of twice the diameter, unconfined charges[31, 41]: Diameter (mm) / ρ (g cm^{-3}) / VoD (m/s) 14.5 / 1.81 / no go 16.0 / 1.80 / 7,650 20.0 / 1.81 / 7,800 25.0 / 1.80 / 7,820 30.0 / 1.80 / 7,860 7,940 (@ 1.77 g cm^{-3}, Cu tube)[31]

			7,790 (@ 1.78 g cm^{-3}, H_2O test variant)[31] 7,800 (@ 1.78 g cm^{-3}, H_2O test variant)[31] 7,860 (@ 1.8 g cm^{-3}, unconfined charges)[31] 7,940 (1.77 g cm^{-3}, confined in Cu tube used in cylinder test)[31, 41] 8,001 (@ 1.82 g cm^{-3})[34] 7,790 (@ 1.78 g cm^{-3}, mod. aquarium test)[41] 7,780 (@ 1.78 g cm^{-3}, mod. aquarium test)[41] 8,590 (@ 1.91 g cm^{-3})[42] 7,400 (@ 1.69 g cm^{-3}, 4 mm outer diameter Cu sheath)[42] 7,770 (@ 1.71 g cm^{-3}, 4 mm outer diameter Cu sheath)[42] 8,220 (@ 1.87 g cm^{-3})[55] 8,180 (@ 1.87 g cm^{-3})[55] 8,200 (@ 1.86 g cm^{-3})[55] 8,090 (@ 1.83 g cm^{-3})[55] 8,020 (@ 1.8 g cm^{-3})[55]
V_0 [L kg^{-1}]		908 (@ 1.90 g cm^{-3}, calcd., LOTUSES)[61]	855 [8]
Critical diameter [cm]	13–25 mm[20], 16.0 mm[31], 16.0 mm (mean particle size = 130 µm, charges pressed @ 1.8 g cm^{-3})[31, 41]		
Critical temperature [K]	829[49], Henkin critical T = 237 °C[49], Henkin critical T = 216 °C[49], 828.5 (est., *Joback-Stein* method)[60], 1,291.6 (*Valderrama-Alveraz* method)[60]		

Critical pressure [bar]	86.05 (est., Joback-Stein method)[60], 145.15 (Valderrama-Alveraz method)[60]
Plate dent test	5.72 mm (no crater)[34]
Gap test	Charge $\rho = 1.83$ g cm^{-3}, gap test >50 kbar[15, 34]
LSGT [cm]	$m_{50\%}$ = 260 cards (NOL LSGT, ρ not specified cf. RDX = 310 cards, TATB = 190 cards)[42], 260 (0.19 mm polymethylmethacrylate attenuation discs)[49]
5 s explosion T [°C] Explosion T [°C] Ignition T [°C] Autoignition T [°C]	 284 (DTA/TG @ 6 °C/min)[15], 236 (DTA/TG @ 6 °C/min)[34] 258 (recryst. NTO, MRL data)[42, 49], 270 (unrecryst. NTO, MRL data)[42], 237 (US data, @ 0.64 mm, recryst. NTO)[42], 280 (recryst. NTO, French data, SNPE)[42, 49] 538.2 K[49]
Small-scale autoignition test, Thiokol) [°C]	234[36]
Thermal stability [no. moles (g) per mole NTO/ no. h]	@ 120 °C: 0/22, 0/72[22] @ 220 °C: 2.13/22, 2.2/72[22] @ 320 °C: 2.4/22, 2.3/72[22]
Vacuum stability test [cm^3/h]	0.0 mL/5 g @ 120 °C, 40 h[17], 0.2 mL/g/48 h @ 100 °C[18, 29, 49], 0.3 mL/g/48 h @ 120 °C[18], 0.06 mL/g @ 100 °C, 20 h[35, 49], 0.05 cm^3/g @ 110 °C, 20 h ($\rho = 1.93$ g cm^{-3})[44], 0.0 mL/g/120 °C/40 h (recryst. NTO, MRL data)[42, 49], 0.3 mL/g/120 °C/48 h (recryst. NTO, US data)[42, 49], 1.45 cm^{3}g^{-1}/150 °C/193 h[49], 1.7 cm^3/g/150 °C/193 h[49], stable 0.0 cm^3/g/150 °C/193 h[49], 0.2139 mL/5 g @ 94 °C for 48 h[59]
Vapor pressure [atm @ °C]	0.03–0.3 @ 230–270 °C[45]
Burn rate [mm/s]	Window constant-pressure bomb, 1.5 L in 0.1–40 MPa pressure interval, samples prepared as pressed cylinders of 0.98 TMD (1.87 g cm^{-3}) confined in transparent acrylic tubes of 7 mm inner diameter prior to pressing[45]: 0.3 mm/s @ 0.4 MPa.
Solubility [g/mL]	0.72 g dissolve in 100 mL H_2O @ 4.85 °C[42, 49], 1.28 g dissolve in 100 mL H_2O @ 18.95 °C[42, 49], 2.6 g dissolve in 100 mL H_2O @ 43.3 °C[42, 49], approx.. 10 g dissolve in 100 mL H_2O @ 100 °C[42, 49], 1.68 g dissolve in 100 mL acetone @ 18.95 °C[42, 49], 0.28 g dissolve in 100 mL ethyl acetate @ 18.95 °C[42, 49], <0.02 dissolve in 100 mL CH_2Cl_2 @ 18.95 °C[42, 49], 18 g/L in acetone[49], 625 g/L in DMSO[49], 16,642.0 mg/L in H_2O @ 25 °C[50], can be reycryst. from boiling water[51], 49 g/l H_2O[58], soluble in most organic solvents[58], 9.99 g/L in H_2O @ 11.5 K[60], 19.99 g/L in H_2O @ 33.9 °C[60], 7.56 g/L in H_2O @ 298.15 K (est., Klopman method)[60], 9.97 g/L in H_2O @ 298.15 K (est., COSMOtherm method)[60]

<table>
<tr><td></td><td>Values using density method[46]:

<table>
<tr><td rowspan="2">Solvent</td><td colspan="4">X[$g_{NTO}/g_{solvent}$]</td></tr>
<tr><td>@ 20 °C</td><td>@ 40 °C</td><td>@ 60 °C</td><td>@ 80 °C</td></tr>
<tr><td>H_2O</td><td>0.021</td><td>0.035</td><td>0.063</td><td>0.120</td></tr>
<tr><td>Ethanol</td><td>0.331</td><td>0.644</td><td>1.143</td><td></td></tr>
</table>

Aqueous solubility: 7.46 g/L[49], 9.97 g/L @ 25 °C[49], 49 g/L[49]

Solubility (g/ 1,000 g nitric acid) in 80.5% nitric acid[49]: 3 g @ 5 °C, 4 g @ 10 °C, 5 g @ 18 °C, 6 g @ 38 °C[49]
Solubility (g/1,000 g nitric acid) in 33.3% nitric acid[49]: 4 g @ 45 °C, 5 g @ 60 °C, 6 g @ 70 °C, 7 g @ 75 °C[49]
Solubility (g/1,000 g nitric acid) in 51.8% nitric acid[49]: 3 g @ 38 °C, 4 g @ 50 °C, 5 g @ 60 °C, 7 g @ 78 °C[49]</td></tr>
<tr><td>Photosensitivity</td><td>Solid samples of NTO decompose using 7 ns pulses from a Nd:YAG laser applied normal to the surface of the pellet @ 266 nm wavelength[49], Complete dec. of 150 mg/L NTO with 0.4 g/L TiO_2 in 3 h on irradiation with 290 nm[49], no significant dec. observed in absence of TiO_2[49]</td></tr>
<tr><td>Compatibility</td><td>Impact sensitivity shows NTO sensitized by 60 µm Pyrex powder[33], polycarbonate[33], polystyrene[33], or PMMA[33] – ignition occurs @ 1.30 m drop height, if one of the sensitizers was distributed throughout the layer then almost all of the explosive was consumed[33]

H_2O content in mass (%) (Karl-Fischer method) and mass loss on storage[37]:

<table>
<tr><td>Storage time @ 65.5 °C</td><td>K-F value (mass %)</td><td>Mass loss after storage (%)</td></tr>
<tr><td>0</td><td>0.15</td><td>–</td></tr>
<tr><td>2 months</td><td>0.13</td><td>0.04</td></tr>
<tr><td>4 months</td><td>0.07</td><td>0.09</td></tr>
</table>

VST of NTO/TNAZ (60/40) @ 110 °C, 20 h, vol. of gas evolved = 0.02 cm^3/g[44]</td></tr>
<tr><td>pK_a</td><td>3.67[43, 47, 49], 3.78[49], 4.7 ± 0.20[49], 3.76[50]</td></tr>
<tr><td>Heat of sublimation [kcal/mol]</td><td>26.4[45], enthalpy of subl = 110.5 kJ/mol[49]</td></tr>
<tr><td>Heat of melting [kcal/mol]</td><td>6.7[45], enthalpy of fusion = 28.0 kJ/mol[49], enthalpy of fusion ΔH_m = 20.17 kJ/mol[49, 60], enthalpy of fusion = 27 kJ/mol[49, 60], ΔH_m = 92.8 kJ/mol [60]</td></tr>
<tr><td>Heat of evaporation [kcal/mol]</td><td>19.7[45], enthalpy of vap = 82.4 kJ/mol[49]</td></tr>
</table>

<table>
<tr><td>Decomposition activation energy [kcal/mol]</td><td>40.7 (110–140 °C interval, open vessel, TGA)[45], 77–88 (200–260 °C interval, open vessel, TGA)[45], 44.5 (229–246 °C interval, open vessel, TGA)[45], 48.8 (in H_2O soln.)[45], 38.4 (in acetone soln.)[45]</td></tr>
<tr><td>Flame T in combustion wave</td><td>T_s = surface temperature, T_1 = temperature of first flame, T_2 = temperature of second flame[45]:

<table><tr><th>Characteristic pressure (MPa)</th><th>T_s (K)</th><th>T_1 (K)</th><th>T_2 (K)</th><th>Adiabatic flame T (K)</th></tr><tr><td>0.4</td><td>645</td><td>980</td><td>1,500</td><td>2,225</td></tr><tr><td>0.5</td><td>639 ± 15</td><td>1,030 ± 20</td><td>1,667 ± 61</td><td>2,224</td></tr><tr><td>0.6</td><td>624</td><td>1,100</td><td>1,750</td><td>2,224</td></tr><tr><td>1.1</td><td>677 ± 10</td><td>1,150</td><td>1,780</td><td>2,224</td></tr><tr><td>1.6</td><td>673</td><td>1,075</td><td>1,975</td><td>2,225</td></tr><tr><td>2.1</td><td>700 ± 18</td><td>–</td><td>1,980 ± 20</td><td>2,225</td></tr></table></td></tr>
<tr><td>Gurney energy [kJ/kg]</td><td>2,580 (est. based on cylinder test results)[48]</td></tr>
<tr><td>Particle sizes</td><td>Large, rod-like, jagged crystals which tend to agglomerate on recryst. from H_2O[47], finely divided particles with 5.7 m^2/cm^3 surface areas obtainable using solvent/nonsolvent method (Kayser)[47], nano-NTO obtained using spray-freezing into liquid (SFL) method – elongated shape, 70–90 nm width, 200–300 nm length 18.1 m^2/g specific surface area[47]</td></tr>
<tr><td>Log K_{ow}</td><td>0.82–1.19[49], 0.37–1.03[50], –0.82 (est., Broto method)[60], –1.19 (est. COSMOtherm method)[60]</td></tr>
<tr><td>Log K_{oc}</td><td>1.0–4.24 @ pH 10–1[49], 1.1 (measured)[50], 2.1 (est.)[50]</td></tr>
<tr><td>Heat capacity [J g^{-1} K^{-1}]</td><td>1.46[49], standard molar heat capacity = 141.53 J/mol/K[49]

Ideal gas heat capacity[49]:

<table><tr><th>T (K)</th><th>C_p (cal mol^{-1} K^{-1})</th><th>T (K)</th><th>C_p (cal mol^{-1} K^{-1})</th></tr><tr><td>300</td><td>28.1</td><td>2,000</td><td>58.1</td></tr><tr><td>400</td><td>34.2</td><td>2,500</td><td>59.2</td></tr><tr><td>500</td><td>39.1</td><td>3,000</td><td>59.9</td></tr><tr><td>600</td><td>42.9</td><td>3,500</td><td>60.3</td></tr><tr><td>800</td><td>48.1</td><td>4,000</td><td>60.6</td></tr><tr><td>1,000</td><td>51.4</td><td>4,500</td><td>60.8</td></tr><tr><td>1,500</td><td>55.9</td><td>5,000</td><td>61.0</td></tr></table></td></tr>
<tr><td>Biodegradation</td><td>Biodegradation by Bacillus licheniformis[49]</td></tr>
<tr><td>BIC test</td><td>NTO with 10% RDX[54]: $<dp/dt \geq 2.2$ psi/μs[54]</td></tr>
</table>

	α-NTO[3]	β-NTO[4]	β-NTO[4]	β-NTO[4]	β-NTO[4]	β-NTO[4]	β-NTO[58]	α-NTO[58]
Chemical formula	$C_2H_2N_4O_3$	$C_2H_2N_4O_3$	$C_2H_2N_4O_3$	$C_2H_2N_4O_3$	$C_2H_2N_4O_3$	$C_2H_2N_4O_3$	$C_2H_2N_4O_3$	$C_2H_2N_4O_3$
Molecular weight [g mol^{-1}]	130.08	130.08	130.08	130.08	130.08	130.08	130.08	130.08
Crystal system	Triclinic*	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Triclinic
Space group	*P*–1	$P2_1/c$ (no. 14)	$P2_1/c$ (no. 14)	$P2_1/c$ (no. 14)	$P2_1/c$ (no. 14)	$P2_1/c$ (no. 14)	$P2_1/c$ (no. 14)	*P*–1
a [Å]	5.1233(8)	9.3129(4)	9.3185(4)	9.3220(4)	9.3233(4)	9.3207(4)	9.326(2)	5.12
b [Å]	10.314(2)	5.4458(2)	5.4615(2)	5.4791(2)	5.4977(2)	5.5215(2)	5.515(2)	10.30
c [Å]	17.998(3)	9.0261(4)	9.0475(3)	9.0685(3)	9.0885(3)	9.1102(3)	9.107(2)	17.9
α [°]	106.610 (2)	90	90	90	90	90	90	106.7
β [°]	97.810(2)	101.464(2)	101.3320(10)	101.1820(10)	101.0190(10)	100.8700(10)	100.77(2)	97.7
γ [°]	90.130 (2)	90	90	90	90	90	90	90.2
V [Å^3]	902.1(2)	448.64(3)	451.48(3)	454.39(3)	457.26(3)	460.44(3)	460.2(2)	
Z	8	4	4	4	4	4	4	8
ρ_{calc} [g cm^{-3}]	1.916	1.926	1.914	1.901	1.889	1.876	1.878	1.92
T [K]	298	100	150	200	250	298	294	
							crystal from cooling a hot aq. NTO soln.	

* The crystals of α-NTO measured in ref.[3] are multiple twins that can be rationalized by stacking faults of identical layers. Transformation of the triclinic primitive cell gives an *I*-centered cell with space group *I*-1, nearly orthorhombic metrics, $Z = 16$, $\alpha = 90.030°$, $\beta = 89.600°$, $\gamma = 89.848°$; If *I*-centered cell is idealized to show an orthorhombic metric then $a = 5.1233$, $b = 10.314$, $c = 34.143$[52].

Recrystallizes from H_2O as large, rod-like, jagged crystals which tend to agglomerate[47], finely divided particles with 5.7 m^2/cm^3 surface areas obtainable using solvent/nonsolvent method (*Kayser*)[47], nano-NTO obtained using SFL method, nano-NTO shows same diffraction pattern as micro-NTO which is α-NTO[47], α-NTO obtained by slow cooling of hot aqueous soln. followed by refrigeration (long needles)[49], β-NTO obtained by recryst. from MeOH or mixed EtOH/CH_2Cl_2, or small quantities by cooling hot aqueous soln.[49], β-NTO only found in recryst. product of NTO from MeOH/CH_2Cl_2 or EtOH/CH_2Cl_2 mixture, no solvent found for producing large enough quantities for preliminary sensitivity tests[58]

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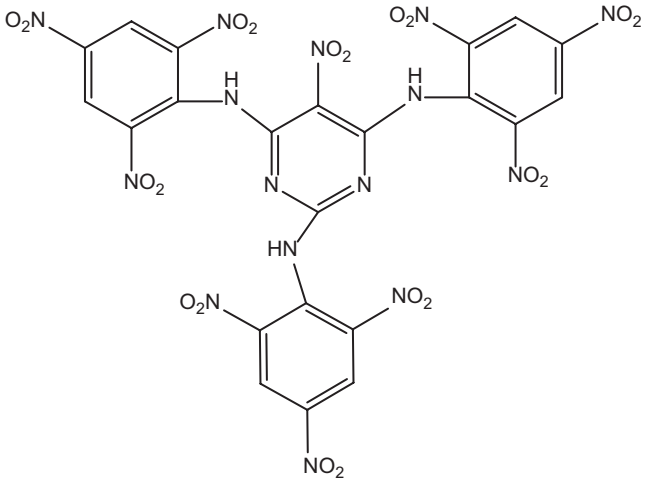
5-Nitro-2,4,6-tris(picrylamino)pyrimidine

Name [German, acronym]: 5-Nitro-2,4,6-tris(picrylamino)pyrimidine [NTPP]
Main (potential) use: Thermally stable explosive[1]
Structural formula:



	NTPP		
Formula	$C_{22}H_9N_{15}O_{20}$		
Molecular mass [g mol^{-1}]	803.40		
Appearance at RT			
IS [J]			
FS [N]			
ESD [J]			
N [%]	26.15		
$\Omega(CO_2)$ [%]	−56.76		
$T_{m.p.}$ [°C]			
$T_{dec.}$ [°C]			
ρ [g cm^{-3}]			
Heat of formation			
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.

$-\Delta_{ex}U^{o}$ [kJ kg^{-1}]			
T_{ex} [K]			
$p_{C\text{-}J}$ [kbar]			
VoD [m s^{-1}]			
V_0 [L kg^{-1}]			

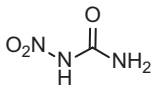
[1] S. R. Ahmad, M. Cartwright, *Laser Ignition of Energetic Materials*, John Wiley and Sons Ltd., **2015**.

Nitrourea

Name [German, acronym]: Nitrourea, 1-nitrourea, *N*-nitrocarbamide [nitroharnstoff, NUr]

Main (potential) use:

Structural formula:



	Nitrourea	
Formula	$CH_3N_3O_3$	
Molecular mass [g mol^{-1}]	105.05	
Appearance at RT	Colorless platelets from EtOH/Et_2O[9], pearly leaflets[13], platelets (from EtOH and petrol ether)[17]	
IS [J]	18 in (incomplete explosion, P.A., 2 kg mass, cf. 14 in for TNT)[9]	
N [%]	40.00	
$\Omega(CO_2)$ [%]	−7.61	
$T_{m.p.}$ [°C]	154–159[1], 158.4–158.8 (dec.)[9], 146–153 (dec.)[13], 158.4–158.8 (pure nitrourea)[13]	
$T_{dec.}$ [°C]	~140[10], 153–155 (dec., no melting, mpt. apparatus, glass capillary)[10], 158.4–158.8[17]	
ρ [g cm^{-3}]	1.557 (@ 293 K)[2], 1.73[10]	
Heat of formation	−281 kJ/mol ($\Delta_f H°$)[3], − 2,688.4 kJ/kg ($\Delta_f H°$)[4], −2,556.4 kJ/kg[5], −614.3 kcal/kg (energy of form.)[9], −639.7 kcal/kg (enthalpy of form.)[9], −59.37 ± 0.15 kcal/mol ($\Delta H_f°$)[14], 1,245 kcal/kg[15], −282.3 kJ/mol (enthalpy of form., exptl.)[18], −281.7 kJ/mol (enthalpy of form., calcd., emp.)[18], −226.6 kJ/mol (enthalpy of form., calcd., S-D method)[18]	
Heat of combustion	133.56 cal/mol[9], −129.56 ± 0.15 cal/mol[14], 1,245 kcal/kg (@ C^V)[15]	
	Calcd. (EXPLO5 5.04)	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]	3,347	800 cal/kg [H_2O (g)][7] 3,865[8] Heat of explosion = 789 kcal/kg[9]
T_{ex} [K]	2,744	

$p_{C\text{-}J}$ [kbar]	180	
VoD [m s^{-1}]	7,150 (@ TMD)	
V_0 [L kg^{-1}]	878	853[6, 8, 9]

Trauzl test [cm^3, % TNT]	105% TNT[12], 310 cm^3[9, 16], 320[16], 94% PA[9]
Sand test [g]	28–30 g (0.4 g nitrourea sample)[9]
Initiation efficiency	Can be detonated by no. 8 MF cap[9]
Thermal stability	Explosion hazard when exposed to heat[9]
Solubility [g/mL]	Freely soluble in acetone, acetic acid, EtOH[9], slightly soluble in benzene, $CHCl_3$, petroleum ether[9], soluble in hot EtOH[13], crystallizes on cooling EtOH soln.[13], sparingly soluble in benzene, Et_2O, $CHCl_3$[13], soluble in hot water but aqueous solns. are unstable[17], freely soluble in acetone, EtOH, acetic acid[17], sparingly soluble in petrol ether, $CHCl_3$, benzene[17]
Compatibility	Can react vigorously with oxidizing materials[9], spontaneous dec. in presence of moisture[13], soluble in hot water but aqueous solns. are unstable[17], almost instantaneous dec. in alkaline solns.[17]
$\Delta H°_{sol}$ [kcal/mol]	7.59 ± 0.02[14]

	Nitrourea[11]
Chemical formula	$CH_3N_3O_3$
Molecular weight [g mol^{-1}]	105.06
Crystal system	Tetragonal
Space group	$P\,4_3\,2_1\,2$ (no. 96)
a [Å]	4.8710(8)
b [Å]	4.8710(8)
c [Å]	32.266(6)
α [°]	90
β [°]	90
γ [°]	90
V [$Å^3$]	756.2
Z	8
ρ_{calc} [g cm^{-3}]	1.823
T [K]	100

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[2] Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© **1994–2017** ACD/Labs).
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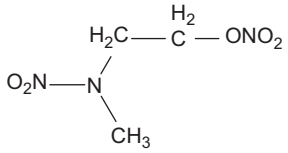
N-(2-Nitroxyethyl)methylnitramine

Name [German, acronym]: *N*-Methyl-*N*-(2-nitroxyethyl)nitramine, [MeNENA]
Main (potential) use: Energetic plasticizers in modern gun propellant formulations[3]

Structural formula:



	MeNENA
Formula	$C_3H_7N_3O_5$
Molecular mass [g mol^{-1}]	165.10
Appearance at RT	Colorless crystalline solid[3]
IS [J]	>90 cm[1], >35 (BAM, dec. but no det.)[3]
FS [N]	120 (BAM, dec. but no det.)[3]
ESD [J]	0.6 (OZM apparatus, dec. but no det.)[3]
N [%]	25.45
Ω(CO_2) [%]	−43.6
$T_{m.p.}$ [°C]	39–40.5 (recryst. product)[1], 36.5–38 (crude product)[1], 38–40[1, 2], 31 (onset, DTA @ 5 °C/min, open glass tube)[3]
$T_{dec.}$ [°C]	218 (exotherm, DSC)[2], 180 (onset exo, DTA @ 5 °C/min, open glass tube)[3]
ρ [g cm^{-3}]	$D^{25}{}_4 = 1.40$ (pycnometer, liq.)[1], $D^{25}{}_4 = 1.53$ (pycnometer, solid)[1], 1.53[2], 1.599 (crystals @ 173 K, X-ray)[3]
Heat of formation	−150.0 kJ/mol ($\Delta_f H°$)[3], 48.68 kcal/mol (−ΔH_f (heat of form. @ standard conditions))[4]
Heat of combustion	Exptl. heat of combustion data[4]:

−$\Delta U_{B/M}$ (cal/g)	−ΔU_B (kcal/mol)	−ΔU_R (kcal/mol @ 1 atm and constant vol.)	−ΔH_R (kcal/mol @ 1 atm and constant pressure)
2,881.82 ± 0.76	475.82	475.17	473.84

	Calcd. (EXPLO5 5.04)	Lit. values	Exptl.
$-\Delta_{ex}U^{o}$ [kJ kg^{-1}]	5,919[3]		
T_{ex} [K]	3,769[3]		
$p_{C\text{-}J}$ [kbar]	259[3]		
VoD [m s^{-1}]	8,050 (@ 1.60 g cm^{-3})[3]		
V_0 [L kg^{-1}]	780[3]		
Thermal stability	No explosion @ 360 °C[1], volatizes rapidly, acid in 65 min @ 135 °C[1]		
Vacuum stability test [cm^3/h]	7.38 cc/5 g/48 h @ 100 °C[1], 100 h required to exceed 12 cc using 2.4 g sample[1]		
Solubility [g/mL]	Recryst. from Et_2O[3]		
Hygroscopicity	0.00% @ 90% RH[1], 0.01% @ 100% RH[1]		
pH	7.2[1]		
Int. test @ 75 °C	0.13% volatility[1], 0.10% volatility[1]		
ΔH_{sub} [kJ/mol]	58.9 (Trouton's rule)[3]		
Berthelot-Rot value (B_R) [kJ•m^3]	11,819[3]		

	Me-NENA[3]
Chemical formula	$C_3H_7N_3O_5$
Molecular weight [g mol^{-1}]	165.12
Crystal system	Monoclinic
Space group	$P2_1/c$ (no. 14)
a [Å]	9.7280(10)
b [Å]	7.3794(7)
c [Å]	11.7814(15)
α [°]	90
β [°]	125.816(11)
γ [°]	90
V [Å^3]	685.82(16)
Z	4

ρ_{calc} [g cm^{-3}]	1.599
T [K]	173
	Recryst. from Et_2O

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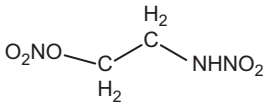
N-(2-Nitroxyethyl)nitramine

Name [German, acronym]: [NENA]
Main (potential) use: Plasticizer
Structural formula:



	NENA		
Formula	$C_2H_5N_3O_5$		
Molecular mass [g mol^{-1}]	151.08		
Appearance at RT	Liquid[1], pale yellow oil[1]		
IS [J]	$H_{50\%}$ = 191 cm[1], $H_{50\%}$ = 107 cm[1]		
N [%]	27.81		
Ω(CO_2) [%]	−15.9		
$T_{m.p.}$ [°C]			
$T_{dec.}$ [°C]			
ρ [g cm^{-3}]			
Heat of formation			
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{ex}U^{o}$ [kJ kg^{-1}]			
T_{ex} [K]			
$p_{C\text{-}J}$ [kbar]			
VoD [m s^{-1}]			
V_0 [L kg^{-1}]			
Thermal stability	No explosion @ 360 °C[1], acid formed in 75 min @ 135 °C[1]		

Volatility	Volatizes rapidly[1]
Solubility [g/mL]	Insoluble in water[1], soluble in/miscible with Et_2O[1]
pH	2.7[1]
Power	133% TNT[1]

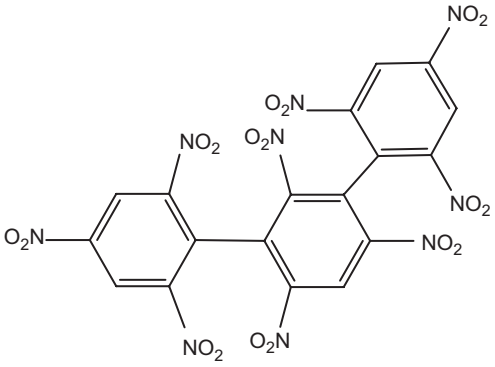
[1] A. T. Blomquist, F. T. Fiedorek, *Nitramines*, US Patent 2,485,855, 25th October **1949**.

Nonanitroterphenyl

Name [German, acronym]: 2,2^{I},2^{II},4,4^{I},4^{II},6,6^{I},6^{II}-Nonanitroterphenyl, tri-1,1′:3,1″-2,4,6-trinitrophenyl, 2,2′,2″,4,4′,4″,6,6′,6″-Nonanitro-1,1′:3′,1″-terphenyl, 2,2′,2″,4,4′,4″,6,6′,6″-Nonanitro-m-terphenyl [Nonanitroterphenyl, NONA]

Main (potential) use: High thermal stability secondary explosive, component of perforators or detonators in downhole well applications, possible spacecraft applications[1], exploding foil initiators, boosters, shaped charges

Structural formula:



	NONA
Formula	$C_{18}H_5N_9O_{18}$
Molecular mass [g mol^{-1}]	635.31
Appearance at RT	Pale yellow solid[15]
IS [J]	20–25 cm[4], 39 cm[4], 9.10[11], H_{50} = 39 cm (2.5 kg mass, type 12 tool)[13], 9.10 (Bruceton method)[14], 39 cm (type 12 tool, 2.5 kg mass, ERL machine)[16]
FS [N]	300 (BAM)[4], FoI (rotary friction) = 2.1[10]
ESD [J]	16.44[20]
N [%]	19.85
Ω(CO_2) [%]	−51.63
$T_{m.p.}$ [°C]	440[3, 8, 10, 12], 440–450 (dec.)[4, 7], does not melt (TG-DSC @ 5 K/min, N_2)[15]
$T_{dec.}$ [°C]	309 (DTA, onset exotherm)[11, 14], 364.8 (TG-DSC @ 5 K/min, N_2)[15]
ρ [g cm^{-3}]	1.78 (crystal)[2, 4, 7, 10], 1.816 (crystal @ 257 K)[15]

Heat of formation	31.6 kcal mol^{-1}[2], −148.2 kJ/mol (calcd.)[15], 27.4 kcal/mol[18], 27.4 kcal/mol ($\Delta H°_f$)[19]		
Heat of combustion	−1,891.2 kcal mol^{-1}[2], $\Delta H°_c$ = −1,891.2 kcal/mol[19]		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{ex}U°$ [kJ kg^{-1}]		4,751 MJ•kg^{-1} (@ TMD, Q_{real})[11, 14]	
T_{ex} [K]		3,780 (@ 1.70 g cm^{-3}, calcd. BKWR)[18] 4,510 (@ 1.70 g cm^{-3}, calcd. BKWS)[18]	
$p_{C\text{-}J}$ [kbar]		255 (calcd., K-J)[2] 26.58 GPa (@ 1.816 g cm^{-3}, calcd., K-J)[15] 241 (@ 1.70 g cm^{-3}, calcd. BKWR)[18] 221 (@ 1.70 g cm^{-3}, calcd. BKWS)[18]	
VoD [m s^{-1}]		7,610 (@ 1.78 g cm^{-3}, calcd., K-J)[2] 7,310 (@ 1.78 g cm^{-3}, calcd. empirical, Rothstein method)[6] 7,600 (@ TMD, calcd., K-J)[11, 14] 7,720.66 (@ 1.816 g cm^{-3}, calcd., K-J)[15] 7,350 (@ 1.70 g cm^{-3}, calcd. BKWR)[18] 7,260 (@ 1.70 g cm^{-3}, calcd. BKWS)[18]	7,560 (ρ not given)[2, 6] 7,560 (@ 1.78 g cm^{-3})[9] 7,400 (@ 1.70 g cm^{-3})[18]
V_0 [L kg^{-1}]			

5 s explosion T [°C] Ignition T [°C]	359[11, 14]
Thermal stability	280 °C (threshold of thermal stability)[11, 14], 87% mass loss in 350–430 °C range[15], max. rate of mass loss at 378.3 °C (–16.89%)[15]
Vacuum stability test [cm^3/days]	0.4 cc/g/h @ 260 °C[4], 0.5 cc/g/h (2 h period) @ 260 °C[16] @ 200 °C (total cm^3 of gas evolved): 0.4/2, 0.8/7, 1.1/14, 1.6/21, 2.0/28, 2.3/35, 2.8/42, 3.2/49, 3.6/56, 3.9/63, 4.3/70, 4.7/77, 5.1/84, 5.4/91[1, 17] @ 175 °C (total cm^3 of gas evolved): 0.1/2, 0.1/7, 0.2/14, 0.2/21, 0.3/28, 0.4/35, 0.5/42, 0.6/49, 0.8/56, 0.9/63, 1.0/70, 1.1/77, 1.2/84, 1.3/91[1] @ 260 °C: 0.43 cc/g gas evolved in 20 min surge, 0.16 cc/g/h for 2 h period, 0.18 cc/g/h for 19 h period[5] 35% dec. of NONA after 78 h @ 260 °C[5]
Vapor pressure [atm @ °C]	Nonvolatile @ 210 °C[4]
Solubility [g/mL]	Soluble in acetone[15]
ΔH_{dec} [kJ/mol]	1,203.28[15]

	NONA[15]
Chemical formula	$C_{18}H_5N_9O_{18}$
Molecular weight [g mol^{-1}]	635.31
Crystal system	Orthorhombic
Space group	*Pbca* (no. 61)
a [Å]	16.8223(11)
b [Å]	11.0573(6)
c [Å]	23.0972(14)
α [°]	90
β [°]	90
γ [°]	90
V [$Å^3$]	4,645.99(50)
Z	8
ρ_{calc} [g cm^{-3}]	1.81644
T [K]	257

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