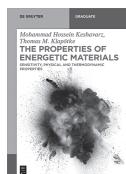


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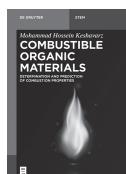


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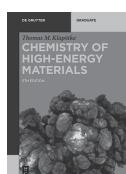


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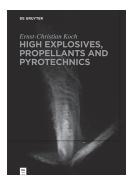
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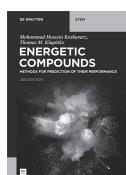
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Thomas M. Klapötke

# Energetic Materials Encyclopedia

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A–D

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# Preface

This book is based on a year-long collaboration between the energetic materials research group at Ludwig Maximilian University Munich (LMU) and the U.S. Army Research Laboratory (ARL), the Army Research Office and the Office of Naval Research (ONR and ONR Global). The need for a unified standard in reporting the sensitivity values and performance parameters of known and in use, as well as new explosives was the driving force behind this project.

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LLM-105	Lawrence Livermore National Laboratory
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Octogen	Lawrence Livermore National Laboratory
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Munich, June 2020

Thomas M. Klapötke

In the following sections, the values in the tables are given in accordance with the following methods/standards (unless reference is specifically given to the original literature in which the values are likely to have been measured using different instrumentation and methods):

impact sensitivity (BAM dropammer, 1 of 6);

friction sensitivity (BAM friction tester, 1 of 6);

electrostatic discharge device (OZM);

decomposition temperature from DSC (heating rate = 5 °C/min);

low-temperature X-ray densities were converted to room temperature values by the volume expansion formula  $\rho_{298K} = \rho_T / (1 + \alpha_v(298 - T_0))$ ;  $\alpha_v = 1.5 \cdot 10^{-4} \text{ K}^{-1}$  or measured by gas pycnometry.

It should also be stressed that impurities or particle size can severely affect the properties (especially the sensitivities) of energetic materials.

For the evaluation of oxidizers, a chamber pressure of 70 bar was assumed with an expansion against both atmospheric pressure (1 bar) and “space conditions” (1 mbar). The combustion conditions were assumed to be isobaric with equilibrium conditions to the throat and frozen to the nozzle exit. As a standard binder, the following formulation was used in all calculations:

6% polybutadiene acrylic acid, 6% polybutadiene acrylonitrile and 2% bisphenol A ether.

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AgN <sub>3</sub>	SA	Silver azide
BaCl <sub>2</sub> O <sub>6</sub>	-	Barium chlorate
BaCl <sub>2</sub> O <sub>8</sub>		Barium perchlorate
BaN <sub>2</sub> O <sub>6</sub>	BN	Barium nitrate
CHN <sub>3</sub> O <sub>6</sub>		Trinitromethane, nitroform
CHN <sub>4</sub> K		Potassium tetrazolate
CHN <sub>5</sub> O <sub>2</sub>	HNT	5-Nitrotetrazole, nitrotetrazole
CH <sub>2</sub> KN <sub>5</sub>		Potassium 5-aminotetrazolate
CH <sub>2</sub> N <sub>4</sub>		Tetrazole
CH <sub>2</sub> N <sub>4</sub> O <sub>5</sub>	DNU	Dinitrourea
CH <sub>2</sub> N <sub>6</sub> O <sub>2</sub>		5-Nitraminotetrazole
CH <sub>2</sub> N <sub>6</sub> O <sub>2</sub>		5-Nitriminotetrazole, 5-nitrimino-1,4 <i>H</i> -tetrazole
CH <sub>3</sub> CIN <sub>4</sub> O <sub>4</sub>	HTz-ClO <sub>4</sub>	1,4 <i>H</i> -Tetrazolium perchlorate
CH <sub>3</sub> NO <sub>2</sub>	NM	Nitromethane
CH <sub>3</sub> NO <sub>3</sub>		Methyl nitrate
CH <sub>3</sub> N <sub>3</sub> O <sub>3</sub>		Nitrourea
CH <sub>3</sub> N <sub>5</sub> O	ATO	1-Aminotetrazol-5-one
CH <sub>3</sub> N <sub>5</sub> O <sub>4</sub>	DNQ	Dinitroguanidine, 1,2-dinitroguanidine
CH <sub>3</sub> N <sub>7</sub> O <sub>4</sub>	HTZ-DN	Tetrazolium dinitramide
CH <sub>4</sub> N <sub>4</sub> O <sub>2</sub>	NQ	Nitroguanidine
CH <sub>4</sub> N <sub>4</sub> O <sub>4</sub>	MEDINA	Methylene dinitramine, <i>N,N</i> -dinitrosomethanediamine
CH <sub>4</sub> N <sub>4</sub> O <sub>4</sub> Cl		5-Aminotetrazolium perchlorate
CH <sub>4</sub> N <sub>4</sub> O <sub>6</sub>	ANF	Ammonium nitroformate
CH <sub>4</sub> N <sub>5</sub> NaO <sub>4</sub>	NANT	Sodium 5-nitrotetrazolate dihydrate
CH <sub>4</sub> N <sub>6</sub>	DAT	Diaminotetrazole, 1,5-diamino-1,2,3,4-tetrazole
CH <sub>4</sub> N <sub>6</sub> O <sub>3</sub>	5-ATN, 5-ATEZN	5-Aminotetrazolium nitrate, aminotetrazolium nitrate, 5-amino-1 <i>H</i> -tetrazole hydronitrate
CH <sub>4</sub> N <sub>8</sub> O <sub>4</sub>	HAT-DN	5-Aminotetrazolium dinitramide
CH <sub>5</sub> CIN <sub>6</sub> O <sub>4</sub>	DAT•HClO <sub>4</sub>	Diaminotetrazolium perchlorate, 1,5-diamino-1 <i>H</i> -tetrazolium perchlorate
CH <sub>5</sub> N <sub>3</sub> O <sub>4</sub>	UN	Uronium nitrate
CH <sub>5</sub> N <sub>5</sub> O <sub>2</sub>	ANQ	Nitroaminoguanidine
CH <sub>5</sub> N <sub>5</sub> O <sub>6</sub>	HNF	Hydrazinium nitroformate
CH <sub>5</sub> N <sub>7</sub> O <sub>3</sub>	DAT-N	Diaminotetrazolium nitrate, 1,5-diamino-1 <i>H</i> -tetrazolium nitrate
CH <sub>5</sub> N <sub>9</sub> O <sub>4</sub>	HDAT-DN	Diaminotetrazolium dinitramide, 1,5-diaminotetrazolium dinitramide
CH <sub>6</sub> N <sub>2</sub>	MMH	Monomethylhydrazine

$\text{CH}_6\text{N}_3\text{O}_4\text{Cl}$		Guanidinium perchlorate
$\text{CH}_6\text{N}_4\text{O}_3$	GuN	Guanidinium nitrate
$\text{CH}_6\text{N}_6\text{O}$	ATO•NH <sub>3</sub>	Ammonium 1-aminotetrazol-5-oneate
$\text{CH}_6\text{N}_6\text{O}_4$	ADNQ	Ammonium dinitroguanidine
$\text{CH}_8\text{N}_5\text{NaO}_3$		Sodium 5-aminotetrazolate trihydrate
$\text{CH}_9\text{N}_7\text{O}_3$	TAGN	Triaminoguanidinium nitrate
$\text{CH}_9\text{N}_9\text{O}_4$	TAGDN	Triaminoguanidinium dinitramide
$\text{CKN}_5\text{O}_2$		Potassium 5-nitrotetrazolate
$\text{CN}_4\text{O}_8$	TNM	Tetranitromethane
$\text{CN}_5\text{O}_2\text{Ag}$		Silver nitrotetrazolate
$\text{C}_2\text{ClCoH}_{12}\text{N}_{14}\text{O}_8$	BNCP	Tetraamine- <i>cis</i> -bis(5-nitro-2 <i>H</i> -tetrazolato) cobalt(III) perchlorate
$\text{C}_2\text{Cu}_2\text{N}_{10}\text{O}_4$	DBX-1	Copper(I) 5-nitrotetrazolate
$\text{C}_2\text{HN}_5\text{O}_9$	TNAА	Tetranitroacetimidic acid
$\text{C}_2\text{H}_2\text{N}_4\text{O}_2$		3-Nitrotriazole, 3-nitro-1,2,4-triazole
$\text{C}_2\text{H}_2\text{N}_4\text{O}_2$		4-Nitrotriazole
$\text{C}_2\text{H}_2\text{N}_4\text{O}_3$	NTO	3-Nitro-1,2,4-triazole-5-one
$\text{C}_2\text{H}_2\text{N}_4\text{O}_8$	TNE	Tetranitroethane
$\text{C}_2\text{H}_2\text{N}_4\text{O}_{12}$		Tetranitroethane
$(\text{C}_2\text{H}_3\text{NO}_3)_n$	PVN	Polyvinyl nitrate
$\text{C}_2\text{H}_3\text{N}_5\text{O}_2$	ANTA	3-Amino-5-nitro-1,2,4-triazole
$\text{C}_2\text{H}_3\text{N}_9$	H <sub>2</sub> BTA	5,5'-Bis(1 <i>H</i> -tetrazolyl)amine
$\text{C}_2\text{H}_4\text{N}_2\text{O}_6$	EGDN	Ethylene glycol dinitrate
$\text{C}_2\text{H}_4\text{N}_4\text{O}$	DAF	3,4-Diaminofurazan
$\text{C}_2\text{H}_4\text{N}_4\text{O}_4$	FOX-7, DADNE	1,1-Diamino-2,2-dinitroethene
$\text{C}_2\text{H}_4\text{N}_6$	DATz	Diaminotetrazine, 3,6-diamino-1,2,4,5-tetrazine
$\text{C}_2\text{H}_4\text{N}_6\text{O}_2$	LAX-112, DATZO <sub>2</sub>	3,6-Diamino-1,2,4,5-tetrazine-1,4-dioxide
$\text{C}_2\text{H}_4\text{N}_{10}$	BTH	5,5'-Bis(1 <i>H</i> -tetrazolyl)hydrazine
$\text{C}_2\text{H}_4\text{N}_{10}$	5,5'-HzTz, HAT	5,5'-Hydrazotetrazole
$\text{C}_2\text{H}_5\text{NO}_2$		Nitroethane
$\text{C}_2\text{H}_5\text{NO}_3$		Ethyl nitrate
$\text{C}_2\text{H}_5\text{N}_3\text{O}_5$	NENA	<i>N</i> -(2-Nitroxyethyl)nitramine
$\text{C}_2\text{H}_5\text{N}_9$	MTX-1	1-[(2E)-3-(1 <i>H</i> -Tetrazol-5-yl)triaz-2-en-1-ylidene]methanediamine
$\text{C}_2\text{H}_6\text{N}_4\text{O}_4$	EDNA	Ethylene dinitramine
$\text{C}_2\text{H}_6\text{N}_8$	DHTz, DHT	1,4-Dihydrazino tetrazine, 3,6-dihydrazine-1,2,4,5-tetrazine
$\text{C}_2\text{H}_6\text{N}_8\text{O}_8$	TNAЕ	<i>N,N,N,N-Tetranitro-1,1,2,2-ethanetetramine</i>
$\text{C}_2\text{H}_6\text{N}_{10}\text{O}_2$	HA.BTO	Hydrazine 5,5'-bitetrazole-1,1'-diolate

**XIV** — Empirical formula, Abbreviations and Names

C <sub>2</sub> H <sub>7</sub> N <sub>3</sub> O <sub>6</sub>		Ethanolamine dinitrate
C <sub>2</sub> H <sub>7</sub> N <sub>5</sub> O <sub>4</sub>		Guanylurea nitrate
C <sub>2</sub> H <sub>7</sub> N <sub>7</sub> O <sub>5</sub>	FOX-12, GUDN	Guanylurea dinitramide
C <sub>2</sub> H <sub>8</sub> Cl <sub>2</sub> N <sub>8</sub> O <sub>8</sub>		3,6-Dihydrazino-1,2,4,5-tetrazine, diperchlorate salt
C <sub>2</sub> H <sub>8</sub> N <sub>2</sub>	sym-DMH	Symmetrical dimethylhydrazine
C <sub>2</sub> H <sub>8</sub> N <sub>2</sub>	UDMH	Unsymmetrical dimethylhydrazine, 1,1-dimethylhydrazine
C <sub>2</sub> H <sub>8</sub> N <sub>8</sub> O	ATO-G	Guanidinium 1-aminotetrazol-5-oneate
C <sub>2</sub> H <sub>8</sub> N <sub>10</sub> O		Tetrazene, 1-amino-1-((1 <i>H</i> -tetrazol-5-yl)-azo)guanidine monohydrate
C <sub>2</sub> H <sub>8</sub> N <sub>10</sub> O <sub>4</sub>	TKX-50	Dihydroxylammonium 5,5-bitetrazole-1,1'-dioxide
C <sub>2</sub> H <sub>9</sub> N <sub>9</sub> O	ATO•AG	Aminoguanidinium 1-aminotetrazol-5-oneate
C <sub>2</sub> H <sub>9</sub> N <sub>9</sub> O <sub>6</sub>	TAGNF	Triaminoguanidinium nitroformate
C <sub>2</sub> H <sub>10</sub> N <sub>4</sub> O <sub>6</sub>	EDD	Ethylenediamine dinitrate
C <sub>2</sub> H <sub>10</sub> N <sub>10</sub> O	ATO•DAG	Diaminoguanidinium 1-aminotetrazol-5-oneate
C <sub>2</sub> H <sub>11</sub> N <sub>11</sub> O	ATO-TAG	Triaminoguanidinium 1-aminotetrazol-5-oneate
C <sub>2</sub> H <sub>15</sub> CoN <sub>10</sub> Cl <sub>2</sub> O <sub>8</sub>	CP	Pentaammine(5-cyanotetrazolato- <i>N</i> <sup>2</sup> )cobalt(III) perchlorate
C <sub>2</sub> HgN <sub>2</sub> O <sub>2</sub>	MF	Mercury fulminate
C <sub>2</sub> HgN <sub>10</sub> O <sub>4</sub>		Mercuric nitrotetrazole, mercury nitrotetrazolate
C <sub>2</sub> K <sub>2</sub> N <sub>12</sub> O <sub>4</sub>	K2DNABT	Potassium 1,1'-dinitramino-5,5'-bistetrazolate
C <sub>2</sub> N <sub>6</sub> O <sub>3</sub>	FTDO	Furazano-1,2,3,4-tetrazine-1,3-dioxide,
C <sub>2</sub> N <sub>6</sub> O <sub>12</sub>	HNE	Hexanitroethane
C <sub>2</sub> N <sub>8</sub> O <sub>4</sub>	TTTO, DTTO	Tetrazino-tetrazine-1,3,6,8-tetroxide
C <sub>3</sub> H <sub>2</sub> N <sub>4</sub> O <sub>4</sub>	DNP	3,4-Dinitropyrazole, 3(5),4-dinitropyrazole
C <sub>3</sub> H <sub>3</sub> N <sub>5</sub> O <sub>4</sub>	DNMT	Dinitromethyltriazole, 1-methyl-3,5-dinitro-1 <i>H</i> -1,2,4-triazole
C <sub>3</sub> H <sub>3</sub> N <sub>5</sub> O <sub>4</sub>	LLM-116, ADNP	4-Amino-3,5-dinitro-1 <i>H</i> -pyrazole
C <sub>3</sub> H <sub>3</sub> N <sub>5</sub> O <sub>4</sub>	5-ADP	5-Amino-3,4-dinitropyrazole
C <sub>3</sub> H <sub>3</sub> N <sub>5</sub> O <sub>10</sub>	TNC-NO <sub>2</sub>	2,2,2-Trinitroethyl nitrocarbamate
C <sub>3</sub> H <sub>3</sub> N <sub>7</sub> O <sub>5</sub>	DNAM	Bis(nitramino)triazinone
C <sub>3</sub> H <sub>4</sub> N <sub>4</sub> O <sub>6</sub>	TNAZ	Trinitroazetidine
C <sub>3</sub> H <sub>4</sub> N <sub>6</sub> O <sub>6</sub>	ATNI	Ammonium 2,4,5-trinitroimidazole
C <sub>3</sub> H <sub>4</sub> N <sub>6</sub> O <sub>7</sub>	K-6	Keto-RDX, 1,3,5-trinitro-1,3,5-triazacyclohexane-2-one
C <sub>3</sub> H <sub>5</sub> NO <sub>4</sub>		Nitroglyceride
C <sub>3</sub> H <sub>5</sub> NO <sub>4</sub> (GLYN)	PGN	PolyGLYN
C <sub>3</sub> H <sub>5</sub> N <sub>3</sub> O (structural unit)	GAP	Glycidyl azide polymer
C <sub>3</sub> H <sub>5</sub> N <sub>3</sub> O <sub>9</sub>	NG	Nitroglycerine
C <sub>3</sub> H <sub>6</sub> N <sub>2</sub> O <sub>6</sub>	PGDN	Propyleneglycol dinitrate
C <sub>3</sub> H <sub>6</sub> N <sub>2</sub> O <sub>6</sub>		Trimethyleneglycol dinitrate

$C_3H_6N_2O_7$		Glycerol 1,2-dinitrate
$C_3H_6N_2O_7$		Glycerol 1,3-dinitrate
$C_3H_6N_6O_3$	TMTA, R-salt, TMTN, TNX	Cyclotrimethylene trinitrosamine
$C_3H_6N_6O_6$	Hexogen, RDX	1,3,5-Trinitro-1,3,5-triazacyclohexane
$C_3H_6N_{10}O_2$	DATr.NTZ	3,4-Diamino-1,2,4-triazolium 5-nitro-tetrazolate
$C_3H_7N_3O_5$	MeNENA	<i>N</i> -(2-Nitroxyethyl)methylnitramine
$C_3H_7NO_3$	IPN	Propyl nitrate
$C_3H_7N_{11}O_2$	DATr.NATZ	3,4-Diamino-1,2,4-triazolium 5-nitramino-tetrazolate
$C_3H_7N_{11}O_2$	HATr.NTZ	3-Hydrazinium-4-amino-1 <i>H</i> -1,2,4-triazolium nitrotetrazolate
$C_3H_8N_4O_4$	DNDA-5, OCPX, DNAP	2,4-Dinitro-2,4-diazapentane
$C_3H_8N_8O_6$	MDN	Melaminium dinitrate
$C_3H_8N_{10}O$	ATO•DATr	3,4-Diamino-1,2,4-triazolium 1-aminotetrazol-5-oneate
$C_3H_8N_{10}O$	DATr.HATZ	3,4-Diamino-1,2,4-triazolium 1-hydroxyl-5-amino- tetrazolate
$C_3H_{10}N_2O_3$	TMAN	Trimethylammonium nitrate
$C_3N_{12}$	TTA, TAT	Cyanuric triazide
$C_4HN_9O_3$	ICM-103	6-Nitro-7-azido-pyrazol[3,4-d][1,2,3]triazine-2-oxide
$C_4H_2N_6O_4$	DNPP	3,6-Dinitropyrazolo[4,3-c]pyrazole
$C_4H_2N_8O_{10}$	TNGU, sorguyl	Tetranitroglycolurile
$C_4H_2N_8O_6$	ICM-101	[2,2'-Bi(1,3,4-oxadiazole)]-5,5'-dinitramide
$C_4H_2N_{12}$	—	3,6-Bis(tetrazol-5-yl)-1,2,4,5-tetrazine
$C_4H_3N_7O_4$		1-Amino-3,6-dinitropyrazolo[4,3-c]pyrazole
$C_4H_4N_6O_4$	ANPZ	2,6-Diamino-3,5-dinitro-1,4-pyrazine
$C_4H_4N_6O_5$	ANPZ-O, LLM-105, NPEX-1, PZO	2,6-Diamino-3,5-dinitropyrazine-1-oxide
$C_4H_4N_6O_6$	DADNB, CL-14	Diamino-dinitrobenzofuroxan, 5,7-Diamino-4,6- dinitrobenzofuroxan
$C_4H_4N_6O_6$	DINGU, DNGU	1,4-Dinitroglycolurile
$C_4H_4N_8O_{14}$	BTNENA, BTNEN, HOX, BTNNA	Bis(trinitroethyl)nitramine
$C_4H_4N_8O_2$	AzoTO	Azotriazolone
$C_4H_4N_8O_3$	AZTO	Azoxytriazolone
$C_4H_4N_8O_3$	DAAF	3,3'-Diamino-4,4'-azoxyfurazan
$C_4H_4N_8O_4$	LLM-119	1,4-Diamino-3,6-dinitropyrazolo[4,3-c]pyrazole
$C_4H_4N_{12}$	DAATz, DAAT	Diaminoazobistetrazine, 3,3'-azobis(6-amino-1,2,3, 5-tetrazine)
$C_4H_4N_{14}$	BTATz	3,6-Bis(1 <i>H</i> -1,2,3,4-tetrazol-5-yl-amino)- <i>s</i> -tetrazine

## XVI — Empirical formula, Abbreviations and Names

$C_4H_5N_5O_4$	NDAPDO	5-Nitro-4,6-diaminopyrimidine-1,3-dioxide
$C_4H_5N_7O_7$	HK-55	2,4,6-Trinitro-2,4,6,8-tetraazabicyclo[3.3.0]-nonane-3-one
$C_4H_5N_8O_9$	K-55, TN550	2,4,6,8-Tetranitro-2,4,6,8-tetraazabicyclo[3.3.0]octane-3-one
$C_4H_6N_4O_6$	DNDMOA, DNDMO, MNO	Dinitrodimethyloxamide
$C_4H_6N_4O_{11}$	NIBTN	Nitroisobutylglycerol trinitrate
$C_4H_6N_4O_{12}$	ETN	Erythritol tetranitrate
$C_4H_6N_6O_4$	NTAPDO, ICM-102, P6NAAA	5-Nitro-2,4,6-triaminopyrimidine-1,3-dioxide
$C_4H_6N_6O_8$	DNNC	1,3,5,5-Tetranitrohexahydropyrimidine, 1,3,5,5-tetranitrohexahydro-1,3-diazine
$C_4H_6N_6O_8$	AMDNNM	Azidomethyl-dinitrooxydimethyl-nitromethane
$C_4H_6N_8O_8$	BCHMX	Bicyclo-HMX, 2,4,6,8-tetranitro-2,4,6,8-tetraazabicyclo[3.3.0] octane
$C_4H_7N_3O_8$	NGIBDN	Nitromethyl propanediol dinitrate
$C_4H_7N_3O_9$	BTTN, BTN	Butanetriol trinitrate
$C_4H_7N_5O_6$	TNP	1,3,5-Trinitrohexahydropyrimidine
$C_4H_8N_2O_6$		Butanediol dinitrate
$C_4H_8N_2O_7$	DEGN, DEGDN, DNDG, DGDN	Diethyleneglycol dinitrate, diglycol dinitrate, nitrodiglycol
$C_4H_8N_4O_8$	DINA	Dioxyethylnitramine dinitrate
$C_4H_8N_8O_8$	Octogen, HMX	1,3,5,7-Tetraza-1,3,5,7-tetranitrocyclooctane
$C_4H_8N_{10}O_8$	MAD-X1, Hx2-DNBTO	Dihydroxylammonium-3,3'-dinitro-5,5'-bis(1,2,4-triazole)-1,1'-diolate
$C_4H_8N_{12}O_6$	DATH	1,7-Diazido-2,4,6-trinitro-2,4,6-triazaheptane
$C_4H_8N_{12}O_{10}$	APX	1,7-Diamino-1,7-dinitrimino-2,4,6-trinitro-2,4,6-triazaheptane
$C_4H_8N_{14}O_2$	HATr.BTO	3-Hydrazinium-4-amino-1 <i>H</i> -1,2,4-triazolium 1 <i>H</i> ,1' <i>H</i> -5,5'-bitetrazole-1,1'-diolate
$C_4H_8N_{16}O_4$	HATr.2NTZ	3-Hydrazinium-4-amino-1 <i>H</i> -1,2,4-triazolium di(5-nitrotetrazolate)
$C_4H_9N_3O_5$	EtNENA	<i>N</i> -Ethyl- <i>N</i> -(2-nitroxyethyl)nitramine
$C_4H_{10}N_4$	DMAZ, CINCH	2-Dimethylaminoethylazide
$C_4H_{10}N_4O_2$	PrNQ	Propyl nitroguanidine
$C_4H_{10}N_4O_4$	DNDA-6	2,4-Dinitro-2,4-diazahexane
$C_4H_{10}N_{18}O_4$	HATr.2NATZ	3-Hydrazinium-4-amino-1 <i>H</i> -1,2,4-triazolium di(5-nitramino-tetrazolate)
$C_4H_{12}N_2O_3$	TeMeAN	Tetramethylammonium nitrate
$C_4H_{12}N_{14}O_4$	2SCZ.BTO	Di(semicarbazide) 5,5'-bitetrazole-1,1'-diolate
$C_4H_{12}N_{18}O_4$	G2DNABT	Bis(guanidinium) 1,1'-dinitramino-5,5'-bitetrazolate

$C_4H_{14}N_9O_8$	DETRA-D	Diethylene-triamine bis-dinitramide
$C_4H_{14}N_{20}O_4$	(AG)2DNABT	Bis(aminoguanidinium) 1,1'-dinitramino-5,5'-bitetrazolate
$C_4H_{14}N_{20}O_6$	(CHZ) <sub>2</sub> DNABT	Bis(diaminouronium) 1,1'-dinitramino-5,5'-bitetrazolate
$C_4N_6O_6$	DNBF	4,4'-Dinitro-3,3'-bifurazan1
$C_4N_8O_8$	DNAF	Dinitrodiazenofuroxan, 4,4'-dinitro3,3'-diazenofuroxan
$C_5H_2N_4O_6$	TNPY	Trinitropyridine
$C_5H_2N_4O_7$	TNPYOX	Trinitropyridine- <i>N</i> -oxide
$C_5H_4N_8O_{10}$	TNPDU	2,4,6,8-Tetranitro-2,4,6,8-tetraazabicyclo[3.3.1]nonane-3,7-dione
$C_5H_6N_6O_4$	TADNP	2,4,6-Triamino-3,5-dinitropyridine
$C_5H_6N_8O_9$	K-56, TN650, TNABN	2,5,7,9-Tetranitro-2,5,7,9-tetraazabicyclo[4.3.0]nonane-8-one
$C_5H_6N_8O_9$	K56	Tetranitro-bicyclo-nonanone
$C_5H_6N_8O_{13}$	BTNEU	Bis(trinitroethyl)urea
$C_5H_6N_{10}O_4$	DNBTM	5,5'-Dinitrimino-3,3'-methylene-1 <i>H</i> -1,2,4-triazole
$C_5H_7N_7O_7$	HK-56	2,5,7-Trinitro-2,5,7,9-tetraazabicyclo [4.3.0]nonane-8-one
$C_5H_8N_2O_8$		Glycerol acetate dinitrate
$C_5H_8N_4O_{12}$	PETN, nitropenta	Pentaerythritol tetranitrate
$C_5H_8N_6O$ (BAMO)	Poly-BAMO	Poly-3,3-bis-(azidomethyl)-oxetane
$C_5H_9NO_4$ (monomer)	Poly-NIMMO	Poly(3-nitratomethyl-3-methyloxetane)
$C_5H_9N_3O$ (AMMO)	Poly-AMMO	Poly-3-azidomethyl-3-methyl-oxetane
$C_5H_9N_3O_8$		Nitroethylpropanediol dinitrate
$C_5H_9N_3O_9$	TMETN, MtrT, MTN	Metriol trinitrate, nitropentaglycerin, trimethylethane trinitrate, pentaglycerol trinitrate, nitrometriol
$C_5H_9N_3O_{10}$	PETRIN	Pentaerythritol trinitrate
$C_5H_9N_7O_2$	DAENP	1,3-Diazido-2-ethyl-2-nitropropane
$C_5H_{10}N_{10}O_9$	ANTTO	1-Azido-8-nitro-2,4,6-trinitro-2,4,6-triazaoctane
$C_5H_{12}N_4O_4$	DNDA-7	3,5-Dinitro-3,5-diazaheptane
$C_5H_{12}N_8O_8$	PETNA	Pentaerythrityl tetranitramine
$C_5H_{12}N_{16}O_2$	2DATr.NATZ	Di(3,4-diamino-1,2,4-triazolium) 5-nitramino-tetrazolate
$C_6HN_3O_6$ (monomer)	PNP	Polynitropolyphenylene
$C_6HN_4O_7K$	KDNP	Potassium 5,7-dinitro-[2,1,3]-benzoxadiazol-4-olate 3-oxide
$C_6HN_5O_{10}$	PNB	Pantanitrobenzene
$C_6H_2KN_3O_7$		Potassium picrate, potassium 2,4,6-trinitrophenate
$C_6H_2N_3O_6Cl$	TNCB	Trinitrochlorobenzene, picryl chloride
$C_6H_2N_4O_5$	DDNP, dinol, diazol, DADNP, DIAZ, DADNPh	2-Diazonium-4,6-dinitrophenolate

**XVIII** — Empirical formula, Abbreviations and Names

C <sub>6</sub> H <sub>2</sub> N <sub>4</sub> O <sub>6</sub>	4,6-DNBF	4,6-Dinitrobenzofuroxan
C <sub>6</sub> H <sub>2</sub> N <sub>4</sub> O <sub>8</sub>	TetNB	Tetranitrobenzene
C <sub>6</sub> H <sub>2</sub> N <sub>6</sub> O <sub>4</sub>	—	Bis(1,2,4-oxadiazolyl) furoxan
C <sub>6</sub> H <sub>2</sub> N <sub>6</sub> O <sub>6</sub>	CL-18	Aminonitrobenzodifuroxan
C <sub>6</sub> H <sub>2</sub> N <sub>6</sub> O <sub>6</sub>	DNBTDO, 5,7-DNBTDO	5,7-Dinitrobenzo-1,2,3,4-tetrazine-1,3-dioxide
C <sub>6</sub> H <sub>2</sub> N <sub>6</sub> O <sub>10</sub>		Pentanitroaniline
C <sub>6</sub> H <sub>2</sub> N <sub>8</sub> O <sub>5</sub>	ANFF-1, LLM-175, ANTF	3-(4-Amino-1,2,5-oxadiazol-3-yl)-4-(4-nitro-1,2, 5-oxadiazol-3-yl)-1,2,5-oxadiazole
C <sub>6</sub> H <sub>3</sub> N <sub>2</sub> O <sub>4</sub> Cl	DNCB	Dinitrochlorobenzene, parazol
C <sub>6</sub> H <sub>3</sub> N <sub>3</sub> O <sub>6</sub>	TNB	Trinitrobenzene
C <sub>6</sub> H <sub>3</sub> N <sub>3</sub> O <sub>7</sub>	PA	Picric acid, 2,4,6-trinitrophenol
C <sub>6</sub> H <sub>3</sub> N <sub>3</sub> O <sub>8</sub>	TNR	Styphnic acid, 2,4,6-trinitroresorcinol
C <sub>6</sub> H <sub>3</sub> N <sub>3</sub> O <sub>10</sub> Pb <sub>2</sub>	Basic LS	Basic lead styphnate, basic lead trinitroresorcinate
C <sub>6</sub> H <sub>3</sub> N <sub>5</sub> O <sub>6</sub>	ADNBF	7-Amino-4,6-dinitrobenzofuroxan
C <sub>6</sub> H <sub>3</sub> N <sub>5</sub> O <sub>8</sub>	TNA	2,3,4,6-Tetranitroaniline
C <sub>6</sub> H <sub>3</sub> N <sub>11</sub> O <sub>4</sub>		6-(4H,8H-Bis[1,2,5]oxadiazolo[3,4-b:3',4'-3]pyrazine-4- yl)-2,4-dioxo-1,2,4,5-tetrazin-3-amine oxolan-2-one
C <sub>6</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub>		Dinitrosobenzene
C <sub>6</sub> H <sub>4</sub> N <sub>4</sub> O <sub>6</sub>	TNA	Trinitroaniline Picramide
C <sub>6</sub> H <sub>4</sub> N <sub>4</sub> O <sub>6</sub> K	KDNBF	Potassium dinitrobenzofuroxan
C <sub>6</sub> H <sub>4</sub> N <sub>6</sub> O <sub>6</sub> K	K CL-14	Potassium salt of CL-14, 5,7-diamino-4,6-dinitrobenzofuroxan, potassium salt
C <sub>6</sub> H <sub>4</sub> N <sub>6</sub> O <sub>8</sub>	—	Bis(1,2,4-oxadiazole)bis(methylene)dinitrate, [3,3'-bis(1,2,4-oxadiazole)]-5,5'-diylbis(methylene) dinitrate
C <sub>6</sub> H <sub>4</sub> N <sub>6</sub> O <sub>16</sub>	BT0x	2,2,2-Bis(trinitroethyl) oxalate
C <sub>6</sub> H <sub>4</sub> N <sub>8</sub> O <sub>3</sub>	—	3,4-Bis(4'-aminofurazano-3') furoxan, 4-[4-(4-amino- 1,2,5-oxadiazol-3-yl)-1,2,5-oxadiazol-3-yl]-1,2,5- oxadiazol-3-amine
C <sub>6</sub> H <sub>4</sub> N <sub>8</sub> O <sub>10</sub>		1,4-Dinitroymethyl-3,6-dinitropyrazolo[4,3-c]pyrazole
C <sub>6</sub> H <sub>4</sub> N <sub>12</sub> O <sub>14</sub>	HHTDD	Hexanitrohexaazatricyclododecanedione, <i>cis-syn-cis</i> -2, 6-dioxo-1,3,4,5,7,8-hexanitrodecahydro-1 <i>H</i> , 5 <i>H</i> -imidazo[4,5- <i>b</i> :4',5'- <i>e</i> ]pyrazine
C <sub>6</sub> H <sub>5</sub> N <sub>3</sub> O <sub>5</sub>		Picramic acid
C <sub>6</sub> H <sub>5</sub> N <sub>5</sub> O <sub>6</sub>	DATB	Diaminonitrobenzene, 2,4,6-trinitro-1, 3-diaminobenzene
C <sub>6</sub> H <sub>5</sub> N <sub>3</sub> O <sub>9</sub> Pb	LS	Lead styphnate
C <sub>6</sub> H <sub>6</sub> N <sub>4</sub> O <sub>4</sub>		Dinitrophenylhydrazine
C <sub>6</sub> H <sub>6</sub> N <sub>4</sub> O <sub>7</sub>	—	Explosive D, ammonium picrate, ammonium-2,4, 6-trinitrophenolate

C <sub>6</sub> H <sub>6</sub> N <sub>4</sub> O <sub>8</sub>	TEX	4,10-Dinitro-2,6,8,12-tetraoxa-4,10-diaza-isowurtzitane
C <sub>6</sub> H <sub>6</sub> N <sub>6</sub> O <sub>6</sub>	TATB	1,3,5-Triamino-2,4,6-trinitrobenzene
C <sub>6</sub> H <sub>6</sub> N <sub>6</sub> O <sub>14</sub>	TNETB	Trinitroethyltrinitrobutyrate
C <sub>6</sub> H <sub>6</sub> N <sub>10</sub> O <sub>10</sub>		<i>Cis-syn-cis</i> -2,6-Dioxo-1,4,7,8-tetranitrodecahydro-1 <i>H</i> , 5 <i>H</i> -diimidazo[4,5- <i>b</i> :4',5'- <i>e</i> ]pyrazine
C <sub>6</sub> H <sub>6</sub> N <sub>12</sub> O <sub>12</sub>	ε-CL-20, HNIW	2,4,6,8,10,12-Hexanitro-2,4,6,8,10,12-hexaaaza-isowurtzitane
C <sub>6</sub> H <sub>7</sub> N <sub>6</sub> NaO <sub>8</sub>	Na[CL-14•2H <sub>2</sub> O]	Sodium 5,7-diamino-4,6-dinitrobenzofuroxane dihydrate
C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> O <sub>8</sub>	ISDN	Isosorbitol dinitrate
C <sub>6</sub> H <sub>8</sub> N <sub>6</sub> O <sub>4</sub>	EGBAA	Ethylene glycol bis(azidoacetate) ester, azido-acetic-acid-2-(2'-azido-acetoxy)-ethyleneester
C <sub>6</sub> H <sub>8</sub> N <sub>6</sub> O <sub>12</sub>	NENO	Dinitrooxyethyloxamide dinitrate
C <sub>6</sub> H <sub>8</sub> N <sub>6</sub> O <sub>16</sub>		3,4-Dideoxy-3,4-dinitro-1,2,5,6-tetra-o-nitrohexitol
C <sub>6</sub> H <sub>8</sub> N <sub>6</sub> O <sub>16</sub>	NEST-1, DNTN	2,3-Dinitro-2,3-bis((nitrooxy)methyl)-butane-1,4-diyl dinitrate, nitrate ester-1, 1,4-dinitrato-2,3-dinitro-2,3-bis(nitratomethylene) butane
C <sub>6</sub> H <sub>8</sub> N <sub>6</sub> O <sub>18</sub>	Nitromannit, MHN	D-Mannitol hexanitrate
C <sub>6</sub> H <sub>8</sub> N <sub>10</sub> O <sub>16</sub>	ZOX	Bis(2,2,2-trinitroethyl- <i>N</i> -nitro) ethylenediamine
C <sub>6</sub> H <sub>9</sub> N <sub>3</sub> O <sub>11</sub>	GLTN	Glycerol nitrolactate dinitrate
C <sub>6</sub> H <sub>10</sub> N <sub>4</sub> O <sub>13</sub>	DGTN	Diglycerol tetranitrate
C <sub>6</sub> H <sub>10</sub> N <sub>6</sub> O <sub>10</sub>	BDNPN	Bis(2,2-dinitropropyl)nitramine
C <sub>6</sub> H <sub>10</sub> N <sub>16</sub> O <sub>2</sub>	2ATr•BTO	Di(1-amino-1,2,3-triazolium) 5,5'-bitetrazole-1,1'-diolate
C <sub>6</sub> H <sub>11</sub> N <sub>3</sub> O <sub>9</sub>	TMPTN	Ethriol trinitrate
C <sub>6</sub> H <sub>12</sub> N <sub>2</sub> O <sub>4</sub>	DMDNB, DMNB	2,3-Dimethyl-2,3-dinitrobutane
C <sub>6</sub> H <sub>12</sub> N <sub>2</sub> O <sub>6</sub>	HMTD	Hexamethylenetriperoxidizediamine
C <sub>6</sub> H <sub>12</sub> N <sub>2</sub> O <sub>8</sub>	TEGDN	Triethyleneglycol dinitrate
C <sub>6</sub> H <sub>12</sub> N <sub>4</sub> O <sub>6</sub>	TMDD	Tetramethylene diperoxide dicarbamide
C <sub>6</sub> H <sub>12</sub> N <sub>6</sub> O <sub>2</sub>	TEGDA, TEG, BATEG	1,2-Bis(2-azidoethoxy)ethane
C <sub>6</sub> H <sub>12</sub> N <sub>16</sub> O <sub>4</sub>	2DATr.DNMZ	Di(3,4-diamino-1,2,4-triazolium) 5-dinitromethyltetrazolate
C <sub>6</sub> H <sub>12</sub> N <sub>22</sub> O <sub>4</sub>	(DATr) <sub>2</sub> DNABT	Bis(3,4-diamino-1,2,4-triazolium) 1,1'-dinitramino-5,5'-bitetrazolate
C <sub>6</sub> H <sub>12</sub> O <sub>4</sub>	DADP	Diacetone diperoxide, 3,3,6,6-tetramethyl-1,2,4,5-tetroxane
C <sub>6</sub> H <sub>13</sub> N <sub>3</sub> O <sub>5</sub>	BuNENA	<i>N</i> -Butyl- <i>N</i> -(2-nitroxyethyl)nitramine
C <sub>6</sub> H <sub>14</sub> N <sub>6</sub> O <sub>6</sub>		Hexamethylenetetramine dinitrate
C <sub>6</sub> H <sub>14</sub> N <sub>6</sub> O <sub>6</sub>	UDN	Urotropinium dinitrate
C <sub>6</sub> H <sub>14</sub> N <sub>22</sub> O <sub>2</sub>	2HATr.DHazo	3-Hydrazino-4-amino-2 <i>H</i> -1,2,4-triazolium 1 <i>H</i> ,1' <i>H</i> -5,5'-azotetrazole-1,1'-diolate
C <sub>6</sub> KN <sub>5</sub> O <sub>7</sub>	KBFNP	Bis(furoxano)nitrophenol, potassium salt

**XX** — Empirical formula, Abbreviations and Names

C <sub>6</sub> N <sub>6</sub> O <sub>6</sub>	BTF	Benzotrifuroxan
C <sub>6</sub> N <sub>6</sub> O <sub>12</sub>	HNB	Hexanitrobenzene
C <sub>6</sub> N <sub>8</sub> O <sub>7</sub>	BNFF-1, LLM-172, BNFF	Bis(nitrofurazano)furan, 3,4-bis(4-nitro-1,2, 5-oxadiazol-3-yl)-1,2,5-oxadiazole
C <sub>6</sub> N <sub>8</sub> O <sub>8</sub>	BNFF, BNFF <sup>0</sup> , DNTF	Bis(nitrofurazano)furoxan
C <sub>6</sub> N <sub>12</sub> O <sub>6</sub>	TATNB	1,3,5-Triazido-2,4,6-trinitrobenzene
C <sub>7</sub> H <sub>2</sub> N <sub>10</sub> O <sub>12</sub>	BTNPM	Bis(3,4,5-trinitropyrazolyl)methane
C <sub>7</sub> H <sub>3</sub> N <sub>3</sub> O <sub>8</sub>	TNBA	Trinitrobenzoic acid
C <sub>7</sub> H <sub>4</sub> N <sub>4</sub> O <sub>7</sub>		2,4,6-Trinitrobenzamide
C <sub>7</sub> H <sub>4</sub> N <sub>4</sub> O <sub>8</sub>	TeNT	Tetranitrotoluene
C <sub>7</sub> H <sub>4</sub> N <sub>4</sub> O <sub>9</sub>	TNBzIN	2,4,6-Trinitrobenzyl nitrate
C <sub>7</sub> H <sub>4</sub> N <sub>8</sub> O <sub>6</sub>	PAT	5-Picrylamino-1,2,3,4-tetrazole
C <sub>7</sub> H <sub>5</sub> N <sub>3</sub> O <sub>6</sub>	TNT	2,4,6-Trinitrotoluene
C <sub>7</sub> H <sub>5</sub> N <sub>3</sub> O <sub>7</sub>	TNAs	Trinitroanisole
C <sub>7</sub> H <sub>5</sub> N <sub>3</sub> O <sub>7</sub>	TNCr	2,4,6-Trinitrocresol
C <sub>7</sub> H <sub>5</sub> N <sub>5</sub> O <sub>8</sub>	CE	Tetryl, N-methyl-N,2,4,6-tetranitroaniline
C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> O <sub>4</sub>	2,4-DNT	2,4-Dinitrotoluene
C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> O <sub>4</sub>	2,6-DNT	2,6-Dinitrotoluene
C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> O <sub>5</sub>	DNAN, 2,4-DNAs	2,4-Dinitroanisole
C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> O <sub>5</sub>	DNCr	Dinitroorthocresol
C <sub>7</sub> H <sub>6</sub> N <sub>10</sub> O <sub>8</sub>	BDNAPM	Bis(3,5-dinitro-4-aminopyrazolyl)methane
C <sub>7</sub> H <sub>7</sub> NO <sub>2</sub>	2-MNT	2-Nitrotoluene
C <sub>7</sub> H <sub>7</sub> NO <sub>2</sub>	3-MNT	3-Nitrotoluene
C <sub>7</sub> H <sub>7</sub> NO <sub>2</sub>	4-MNT	4-Nitrotoluene
C <sub>7</sub> H <sub>7</sub> N <sub>9</sub> O <sub>21</sub>	TNEOF	2,2,2-Trinitroethyl formate
C <sub>7</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub>	MNA	N-Methyl-4-nitroaniline, methyl(4-nitrophenyl)amine
C <sub>7</sub> H <sub>8</sub> N <sub>6</sub> O <sub>7</sub>	GuPicr, GuP	Guanidinium picrate
C <sub>7</sub> H <sub>11</sub> N <sub>9</sub> O <sub>2</sub>	TAP-Ac	Triazidopentaerythrite-acetate
C <sub>7</sub> H <sub>11</sub> N <sub>9</sub> O <sub>2</sub>	TAPE-E	Triazidopivalic-acid-ethylester
C <sub>7</sub> H <sub>12</sub> N <sub>4</sub> O <sub>8</sub>	DNP-4-NAP	2,3-Dinitropropyl-4-nitro-4-azapentanoate
C <sub>7</sub> H <sub>12</sub> N <sub>4</sub> O <sub>10</sub>	BDNPf, DNPFO	Bis(2,2-dinitropropyl)formal
C <sub>7</sub> H <sub>14</sub> N <sub>10</sub> O <sub>14</sub>	TENA-1	1,11-Dinitrato-3,5,7,9-tetranitrazaundecane
C <sub>8</sub> HN <sub>7</sub> O <sub>14</sub>	HpNC	Heptanitrocubane
C <sub>8</sub> H <sub>3</sub> N <sub>11</sub> O <sub>6</sub>		4,6-Di-2(5-nitro-1,2,4-triazole)-5-nitropyrimidine
C <sub>8</sub> H <sub>4</sub> N <sub>16</sub> O <sub>6</sub>		6,6'-(4H,8H-Bis[1,2,5]oxadiazolo[3,4-b:3',4'-e]pyrazine- 4,8-diyl)bis(2,4-dioxo-1,2,4,5-tetrazin-3-amine)
C <sub>8</sub> H <sub>4</sub> N <sub>16</sub> O <sub>6</sub>	ADAAF	Bis[4-aminofurazanyl-3-azoxy]azofurazan
C <sub>8</sub> H <sub>5</sub> N <sub>7</sub> O <sub>6</sub>	PATO	3-Picrylamino-1,2,4-triazole
C <sub>8</sub> H <sub>5</sub> N <sub>13</sub> O <sub>6</sub>	DANTNP	4,6-Bis-(3-amino-5-nitro-1H-1,2,4-triazole-1-yl)-5- nitropyrimidine

C <sub>8</sub> H <sub>5</sub> N <sub>13</sub> O <sub>6</sub>	IHNX	2,4-Bis(5-amino-3-nitro-1,2,4-triazolyl)pyrimidine
C <sub>8</sub> H <sub>6</sub> N <sub>4</sub> O <sub>8</sub>	BIDN	Bis-isoxazole-bis-methylene dinitrate
C <sub>8</sub> H <sub>6</sub> N <sub>4</sub> O <sub>10</sub>	TNPON	Trinitrophenoxyethyl nitrate
C <sub>8</sub> H <sub>6</sub> N <sub>6</sub> O <sub>11</sub>	Pentryl	2,4,6-Trinitrophenylnitraminoethyl nitrate
C <sub>8</sub> H <sub>7</sub> N <sub>3</sub> O <sub>6</sub>	TNX	Trinitroxylene
C <sub>8</sub> H <sub>7</sub> N <sub>3</sub> O <sub>7</sub>	2,4,6-TNPh <sup>t</sup>	Ethyl picrate
C <sub>8</sub> H <sub>7</sub> N <sub>3</sub> O <sub>8</sub>	DNPEN	Dinitrophenoxyethylnitrate
C <sub>8</sub> H <sub>7</sub> N <sub>5</sub> O <sub>8</sub>		Methyltetryl, 2,4,6-trinitro-N-(methylnitro)- <i>m</i> -toluidin
C <sub>8</sub> H <sub>7</sub> N <sub>5</sub> O <sub>8</sub>		Ethyltetryl
C <sub>8</sub> H <sub>12</sub> N <sub>6</sub> O <sub>5</sub>	DEGBA, DEGBAA	Azido-acetic-acid-2-[2'-(2"-azido-acetoxy)-ethoxy]-ethylester
C <sub>8</sub> H <sub>14</sub> N <sub>4</sub> O <sub>10</sub>	BDNPA	Bis(2,2-dinitropropyl)acetal
C <sub>8</sub> H <sub>16</sub> N <sub>10</sub> O <sub>14</sub>	TENA-2	1,12-Dinitro-3,5,8,10-tetranitrazadodecane
C <sub>8</sub> H <sub>18</sub> O <sub>6</sub>	MEKP	2,2'-Peroxydi(butane-2-peroxol), methyl ethyl ketone peroxide
C <sub>8</sub> N <sub>8</sub> O <sub>16</sub>	ONC	Octanitrocubane
C <sub>8</sub> N <sub>16</sub> O <sub>6</sub>	DOATF	3,4:7,8:11,12:15,16-Tetrafurazano-1,2,5,6,910,13,14-octaazacyclohexadeca-1,3,5,7,9,11,13,15-octane-1,10-dioxide
C <sub>9</sub> H <sub>4</sub> N <sub>14</sub> O <sub>8</sub>	LLM-226	4-Diazo-3,5-bis(4-amino-3,5-dinitropyrazol-1-yl) pyrazole
C <sub>9</sub> H <sub>5</sub> N <sub>3</sub> O <sub>7</sub>	PiPE	1,3,5-Trinitro-2-(prop-2-yn-1-yloxy)benzene
C <sub>9</sub> H <sub>7</sub> N <sub>5</sub> O <sub>13</sub>		Glycerol trinitrophenyl ether dinitrate
C <sub>9</sub> H <sub>8</sub> N <sub>4</sub> O <sub>11</sub>	Dinitryl	Glycerol-2,4-dinitrophenyl ether dinitrate
C <sub>9</sub> H <sub>9</sub> N <sub>15</sub> O <sub>18</sub>	TTET	2,4,6-Tris(2,2,2-trinitroethylamino)-1,3,5-triazine
C <sub>9</sub> H <sub>12</sub> N <sub>4</sub> O <sub>13</sub>	FIVONITE	Tetramethylolcyclopentanone tetranitrate
C <sub>9</sub> H <sub>13</sub> N <sub>5</sub> O <sub>15</sub>	FIVOLITE	Nitropentanol, 2,2,5,5-tetramethylolcyclopentanol pentanitrate
C <sub>9</sub> H <sub>18</sub> O <sub>6</sub>	TATP	Triacetonetriperoxide, 3,3,6,6,9,9-hexamethyl-1,2,4,5,7,8-hexaoxocyclononane
C <sub>10</sub> H <sub>4</sub> N <sub>4</sub> O <sub>8</sub>	TENN	Tetranitronaphthalene
C <sub>10</sub> H <sub>4</sub> N <sub>10</sub> O <sub>8</sub>		4-Amino-8-(2,4,6-trinitrophenyl)difurazano[3,4- <i>b</i> :3',4'- <i>e</i> ]pyrazine
C <sub>10</sub> H <sub>5</sub> N <sub>3</sub> O <sub>6</sub>	TNN	Trinitronaphthalene
C <sub>10</sub> H <sub>6</sub> N <sub>2</sub> O <sub>4</sub>	1,5-DNN	1,5-Dinitronaphthalene
C <sub>10</sub> H <sub>6</sub> N <sub>2</sub> O <sub>4</sub>	1,8-DNN	1,8-Dinitronaphthalene
C <sub>10</sub> H <sub>8</sub> N <sub>6</sub> O <sub>14</sub>	BITN	Biisoxazoletetraakis(methyl)nitrate
C <sub>10</sub> H <sub>8</sub> N <sub>8</sub> O <sub>17</sub>	Heptyrl	<i>N</i> -(2,4,6 Trinitrophenyl- <i>N</i> -nitramino)-trimethylolmethane trinitrate
C <sub>10</sub> H <sub>10</sub> N <sub>4</sub> O <sub>8</sub>	BIDNE	[3,3'-Biisoxazole]-5,5'-diylbis(ethane-2,1-diyl)dinitrate
C <sub>10</sub> H <sub>12</sub> N <sub>4</sub> O <sub>12</sub>	DNPF, FUM	Bis(2,2-dinitropropyl) fumarate

**XXII** — Empirical formula, Abbreviations and Names

C <sub>10</sub> H <sub>12</sub> N <sub>10</sub> O <sub>8</sub>	TMNTA	Azido-acetic-acid-3-(2'-azido-acetoxy)-2-(2'-azido-acetoxymethyl)-2-nitropropylester
C <sub>10</sub> H <sub>14</sub> N <sub>4</sub> O <sub>13</sub>	Sixonite	Tetramethylolcyclohexanone tetranitrate
C <sub>10</sub> H <sub>16</sub> N <sub>6</sub> O <sub>19</sub>	DIPEHN, DPEHN	Dipentaerythritol hexanitrate
C <sub>12</sub> H <sub>2</sub> CaK <sub>2</sub> N <sub>6</sub> O <sub>16</sub>	Castyp	Calcium potassium styphnate
C <sub>12</sub> H <sub>4</sub> N <sub>6</sub> O <sub>12</sub>	HNB, HNBP	2,4,6,2',4',6'-Hexanitrobiphenyl
C <sub>12</sub> H <sub>4</sub> N <sub>6</sub> O <sub>12</sub> S	DIPS	2,4,6,2',4',6'-Hexanitrodiphenylsulfide
C <sub>12</sub> H <sub>4</sub> N <sub>6</sub> O <sub>13</sub>	HNDPO	2,4,6,2',4',6'-Hexanitrodiphenyl oxide
C <sub>12</sub> H <sub>4</sub> N <sub>6</sub> O <sub>14</sub>	DIPA	Dipicric acid, 3,3'-dihydroxy-2,2',4,4'6,6'-hexanitrobiphenyl
C <sub>12</sub> H <sub>4</sub> N <sub>6</sub> O <sub>14</sub> S	DIPSO	2,4,6,2',4',6'-Hexanitrodiphenylsulfone
C <sub>12</sub> H <sub>4</sub> N <sub>8</sub> O <sub>8</sub>	Tacot	Tetranitrodibenzo-1,3a,4,6a-tetrazapentalene
C <sub>12</sub> H <sub>4</sub> N <sub>8</sub> O <sub>10</sub>	BTX	5,7-Dinitro-1-picrylbenzotriazole, 1-(2',4',6'-trinitrophenyl)-5,7-dinitrobenzotriazole
C <sub>12</sub> H <sub>4</sub> N <sub>8</sub> O <sub>12</sub>	HNAB	Hexanitroazobenzene
C <sub>12</sub> H <sub>5</sub> N <sub>5</sub> O <sub>8</sub>	TNC	Tetranitrocarbazole
C <sub>12</sub> H <sub>5</sub> N <sub>7</sub> O <sub>12</sub>	HNDP	2,4,6,2',4',6'-Hexanitrodiphenylamine
C <sub>12</sub> H <sub>6</sub> N <sub>8</sub> O <sub>12</sub>	DIPAM	Dipicramide, dipicrylamide, 3,3'-diamino-2,2',4,4',6,6'-hexanitrobiphenyl
C <sub>12</sub> H <sub>9</sub> N <sub>3</sub> O <sub>4</sub>		2,2'-Dinitrodiphenylamine
C <sub>12</sub> H <sub>9</sub> N <sub>3</sub> O <sub>4</sub>		2,4-Dinitrodiphenylamine
C <sub>12</sub> H <sub>9</sub> N <sub>3</sub> O <sub>4</sub>		2,4'-Dinitrodiphenylamine
C <sub>12</sub> H <sub>9</sub> N <sub>3</sub> O <sub>4</sub>		2,6-Dinitrodiphenylamine
C <sub>12</sub> H <sub>9</sub> N <sub>3</sub> O <sub>4</sub>		4,4'-Dinitrodiphenylamine
C <sub>12</sub> H <sub>12</sub> N <sub>18</sub>	HAB	Hexakis(azidomethyl)benzene
C <sub>12</sub> H <sub>14</sub> N <sub>6</sub> O <sub>22</sub> (if complete nitration occurs)	NC	Nitrocellulose
C <sub>12</sub> N <sub>10</sub> O <sub>20</sub>		Decanitrobiphenyl
C <sub>13</sub> H <sub>6</sub> N <sub>8</sub> O <sub>13</sub>		Dipicrylurea, hexanitrocarbanilide
C <sub>13</sub> H <sub>8</sub> N <sub>6</sub> O <sub>10</sub>	PADNT	4-Picrylaminio-2,6-dinitrotoluene
C <sub>13</sub> H <sub>16</sub> N <sub>12</sub> O <sub>8</sub>	PETKAA	Azido-acetic-acid-3-(2'-azido-acetoxy)-2,2-bis-(2'-azido-acetoxymethylpropylester)
C <sub>14</sub> H <sub>4</sub> N <sub>8</sub> O <sub>13</sub>	DPO	2,5-Dipicryl-1,3,4-oxadiazole
C <sub>14</sub> H <sub>4</sub> N <sub>26</sub> O <sub>8</sub>		6,6'-{1,2,4,5-Tetrazine-3,6-diylbis[(4H,8H-bis[1,2,5]oxadiazolo[3,4-b:3',4'-e]pyrazine-8,4-diyl)]}bis(2,4-dioxo-1,2,4,5-tetrazin-3-amine) N,N-dimethylformamide solvate
C <sub>14</sub> H <sub>6</sub> N <sub>6</sub> O <sub>12</sub>	HNS	Hexanitrostilbene
C <sub>14</sub> H <sub>6</sub> N <sub>8</sub> O <sub>14</sub>	HNO	Hexanitroxanilide
C <sub>14</sub> H <sub>7</sub> N <sub>8</sub> O <sub>15</sub>		Hexanitrodiphenylaminoethyl nitrate

$C_{14}H_8N_6O_{10}$	TNO	2,4,2',4'-Tetranitro-oxanilide
$C_{14}H_{10}O_4$		Benzoyl peroxide, dibenzoyl peroxide
$C_{14}H_{16}N_6O_{14}$	BITNE	[3,3'-Biisoxazole]-4,4',5,5'-tetrayltetrakis(ethane-2,1-diyl) tetranitrate
$C_{15}H_9N_7O_{17}$		Hexanitrodiphenylglycerol mononitrate
$C_{15}H_{15}NO_2$		Diphenylurethane
$C_{15}H_{24}N_8O_{26}$	TPEON	Tripentaerythritol octanitrate
$C_{15}H_{30}O_6$	TPTP	Triptanone triperoxide
$C_{16}H_4N_{10}O_{14}$	TKX-55	5,5'-Bis(2,4,6-trinitrophenyl)-2,2'-bi(1,3,4-oxadiazole)
$C_{16}H_4N_{12}O_{14}$		4,8-Bis(2,4,6-trinitrophenyl)-4 <i>H</i> ,8 <i>H</i> -bis([1,2,5] oxadiazolo)[3,4- <i>b</i> :3',4'- <i>e</i> ]pyrazine
$C_{16}H_6N_{10}O_{10}$		4,8-Di(2,4-dinitrophenyl)difurazano[3,4- <i>b</i> :3',4'- <i>e</i> ] pyrazine
$C_{16}H_6N_{12}O_4$	BPABF	4,4'-Bis(picrylamino)-3,3'-bisfurazanyl
$C_{16}H_8N_{18}O_{16}$	BTDAONAB	<i>N,N'</i> -Bis(1,2,4-triazol-3-yl)-4,4'-diamino-2,2',3,3',5,5',6,6'-octanitroazobenzene
$C_{17}H_5N_{13}O_{16}$	PADP	2,6-Bis(picrylazo)-3,5-dinitropyridine
$C_{17}H_7N_{11}O_{16}$	PYX	3,5-Dinitro2,6-bispicrylmino pyridine
$C_{18}H_5N_9O_{18}$	NONA	Nonanitroterphenyl, 2,2 <sup>1</sup> ,2 <sup>11</sup> ,4,4 <sup>1</sup> ,4 <sup>11</sup> ,6,6 <sup>1</sup> ,6 <sup>11</sup> -nonanitroterphenyl
$C_{18}H_6N_8O_{16}$	ONT	Octanitroterphenyl
$C_{21}H_6N_{12}O_{18}$	TPT	2,4,6-Tripicryl-s-triazine
$C_{21}H_9N_{15}O_{18}$	TPM	<i>N</i> <sup>2</sup> , <i>N</i> <sup>4</sup> , <i>N</i> <sup>6</sup> -Tripicrylmelamine
$C_{21}H_{15}N_{21}O_{18}$	PL-1	2,4,6-Tris(3',5'-diamino-2',4',6'-trinitrophenylamino)-1,3,5-triazine
$C_{22}H_9N_{15}O_{20}$	NTPP	5-Nitro-2,4,6-tris(picrylamino)pyrimidine
$C_{22}H_{42}O_4$	DOA	Diocetyl adipate
$C_{24}H_6N_{12}O_{24}$	DODECA	2,2',2 <sup>2</sup> ,2 <sup>2</sup> ,4,4',4 <sup>2</sup> ,4 <sup>2</sup> ,6,6',6 <sup>2</sup> ,6 <sup>2</sup> -Dodecanitroquaterphenyl
$C_{24}H_9N_9O_{18}$	TNTPB, TPB	1,3,5-Tripicrylbenzene
$CuN_3$		Cuprous azide, copper(I) azide
$CuN_6$		Cupric azide, copper(II) azide
$H_4NClO_4$	AP, APC	Ammonium perchlorate
$H_4N_2$		Hydrazine
$H_4N_2O_3$	AN	Ammonium nitrate
$H_5N_2O_4Cl$	HP	Hydrazinium perchlorate
$H_4N_4$	—	Ammonium azide
$H_4N_4O_4$	ADN	Ammonium dinitramide
$H_5N_3O_3$	HZN	Hydrazinium nitrate
$H_8N_{10}Ni$		Bis-hydrazinenickel(II) azide
$H_{12}N_8NiO_6$	NHN, NiHN	Tris-hydrazinenickel(II) nitrate

**XXIV** — Empirical formula, Abbreviations and Names

KClO <sub>3</sub>		Potassium chlorate
KClO <sub>4</sub>		Potassium perchlorate
KNO <sub>3</sub>		Potassium nitrate
KN <sub>3</sub> O <sub>4</sub>	KDN	Potassium dinitramide
N <sub>3</sub> Na		Sodium azide
N <sub>6</sub> Pb	LA	Lead azide
NaClO <sub>3</sub>		Sodium chlorate
NaClO <sub>4</sub>		Sodium perchlorate
NaNO <sub>3</sub>	SN	Sodium nitrate
PbC <sub>6</sub> H <sub>2</sub> N <sub>2</sub> O <sub>6</sub>	PbDNR, 2,4-LDR, LDNR	Lead 2,4-dinitroresorcinol, lead 2,4-dinitroresorcinate
Sr(NO <sub>3</sub> ) <sub>2</sub>		Strontium nitrate

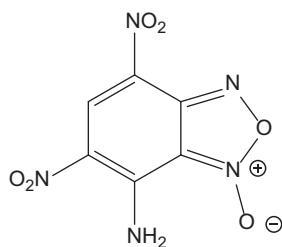
# A

## 7-Amino-4,6-dinitrobenzofuroxan

Name [German, acronym]: 4-Amino-5,7-dinitro-2,1,3-benzoxadiazole 3-oxide  
[7-amino-4,6-dinitrobenzofuroxan, ADNBF]

Main (potential) use: Possible use as thermally stable, insensitive explosive<sup>[2,8]</sup>, promising as an insensitive booster explosive<sup>[1]</sup>

Structural formula:



	<b>ADNBF</b>												
Formula	C <sub>6</sub> H <sub>3</sub> N <sub>5</sub> O <sub>6</sub>												
Molecular mass [g mol <sup>-1</sup> ]	241.12												
Appearance at room temperature (RT)	Thin gold-colored plates <sup>[2]</sup> , orange solid <sup>[2]</sup>												
IS [J]	<p><math>H_{50} = 53 \text{ cm}</math> (B.M., 2.5 kg mass, type 12 tool)<sup>[2,6,7]</sup>, <math>H_{50} = 100 \text{ cm}</math> (24.5 J)<sup>[3]</sup>, <math>H_{50} = 100 \text{ cm}</math> (2.5 kg mass, type 12 tool)<sup>[5]</sup>, <math>H_{30} = 100 \text{ cm}</math> (cf. 75 cm for TNT, B.M.)<sup>[8]</sup>, <math>H_{50\%} = 100 \text{ cm}</math> (2.5 kg mass, type 12 tool, 35 mg sample in conical pile, 1 in<sup>2</sup> garnet paper)<sup>[13]</sup>, <math>H_{50\%} = 100 \text{ cm}</math> (2.5 kg mass)<sup>[14]</sup></p> <p>Rotter impact data: 27 mg sample, Bruceton method, 25 drop run to obtain <math>H_{50\%}</math>; initiation criteria = 1 mL gas evolved or 0.5 mL accompanied by smoke or evidence of burning in the sample<sup>[12]</sup>:</p> <table border="1"><thead><tr><th colspan="2">Rotter impact data</th><th colspan="2">US data</th></tr><tr><th>F of I</th><th>Gas evolved (mL)</th><th>NSWC/NOL, ERL type 12</th><th>NWC B.M. type 12</th></tr></thead><tbody><tr><td>60</td><td>13.0</td><td></td><td>53, 100</td></tr></tbody></table>	Rotter impact data		US data		F of I	Gas evolved (mL)	NSWC/NOL, ERL type 12	NWC B.M. type 12	60	13.0		53, 100
Rotter impact data		US data											
F of I	Gas evolved (mL)	NSWC/NOL, ERL type 12	NWC B.M. type 12										
60	13.0		53, 100										

	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 ( $X$ ), $H_{50\%} = 82$ cm, data from <sup>[12]</sup> :				
	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	1	0.05	4.6	12.9
	1.0	18	0.9	5.7	18.1
	1.5	20	1	12.4	36.1
	2.0	20	1	14.8	44.4
	2.5	20	1	14.3	44.8
$N$ [%]	29.1				
$\Omega(\text{CO}_2)$ [%]	-49.8				
$T_{\text{m.p.}}$ [°C]	270 (dec., DSC @ 10 °C/min) <sup>[2,6,8]</sup> , 270 <sup>[7]</sup>				
$T_{\text{dec.}}$ [°C]	274 (exo, DSC @ 10 °C/min) <sup>[2]</sup>				
$\rho$ [g cm <sup>-3</sup> ]	1.902 (crystal) <sup>[1]</sup> , 1.902 ± 0.008 (gas compression pycnometer) <sup>[2,8]</sup> , 1.90 (crystal) <sup>[6]</sup> , 1.90 <sup>[7,13]</sup>				
Heat of formation	36.79 ± 0.72 kcal mol <sup>-1</sup> <sup>[2,8]</sup> , 133.0 kcal/kg (enthalpy of form.) <sup>[4]</sup> , 86.3 kJ/mol (enthalpy of form., expt.) <sup>[11]</sup> , 169.9 kJ/mol (enthalpy of form., calcd., emp.) <sup>[11]</sup> , 116.6 kJ/mol (enthalpy of form., calcd., S-D method) <sup>[11]</sup>				
	Calcd. (EXPLO5 6.04)		Lit. values		Exptl.
$-\Delta_{\text{ex}}U^\circ$ [kJ kg <sup>-1</sup> ]			1,131 kcal/kg (@ 1.730 g cm <sup>-3</sup> , calcd.) [H <sub>2</sub> O vapor] <sup>[4]</sup>	1,110 kcal/kg (@ 1.730 g cm <sup>-3</sup> ) [H <sub>2</sub> O vapor] <sup>[4]</sup>	
$T_{\text{ex}}$ [K]					
$p_{\text{C-J}}$ [kbar]			282 (@ TMD, calcd., R-P method) <sup>[2]</sup>		
			280 (@ 1.88 g cm <sup>-3</sup> , calcd.) <sup>[13]</sup>		

VoD [ $\text{m s}^{-1}$ ]		7,910 (@ TMD, calcd. R-P method) <sup>[2]</sup>  7,910 (@ 1.90 $\text{g cm}^{-3}$ ) <sup>[7]</sup>  7,890 (@ 1.88 $\text{g cm}^{-3}$ , calcd.) <sup>[13]</sup>	7,814 (@ 92.0% TMD, 4.05 mm charge diameter) <sup>[1]</sup>  7,306 (@ 92.0% TMD, 2.025 mm charge diameter) <sup>[1]</sup>  7,810 (@ 89.9% TMD, 5.95 mm charge diameter) <sup>[1]</sup>  7,718 (@ 89.9% TMD, 4.05 mm charge diameter) <sup>[1]</sup>  7,094 (@ 89.9% TMD, 2.025 mm charge diameter) <sup>[1]</sup>  7,426 (@ 87.5% TMD, 5.95 mm charge diameter) <sup>[1]</sup>
$V_0$ [ $\text{L kg}^{-1}$ ]			
Critical diameter [cm]		$d_c < 2.0$ mm (@ 92.0% TMD, est. value from VoD values) <sup>[1]</sup> , $2.0 > d_c < 1.5$ mm (@ 89.9% TMD, est. value from VoD values) <sup>[1]</sup>	
Solubility [g/mL]		Soluble in $\text{CH}_3\text{CN}$ <sup>[2]</sup> , recryst. from $\text{CH}_3\text{CN}$ <sup>[2]</sup> , recryst. from 70% nitric acid <sup>[2]</sup>	

<b>ADNBF<sup>[9,10]</sup></b>	
Chemical formula	$\text{C}_6\text{H}_3\text{N}_5\text{O}_6$
Molecular weight [g mol <sup>-1</sup> ]	241.1
Crystal system	Monoclinic
Space group	$P2_1$
$a$ [\mathring{A}]	11.959(7)
$b$ [\mathring{A}]	9.863(6)
$c$ [\mathring{A}]	7.180(4)
$\alpha$ [°]	90
$\beta$ [°]	98.131(1)
$\gamma$ [°]	90

$V$ [Å <sup>3</sup> ]	838.4(9)
$Z$	4
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.910
$T$ [K]	293

Crystal morphologies from cosolvent recrystallization<sup>[9]</sup>: cosolvent systems change the ADNBF crystal morphology from needle-like to plate-like<sup>[9]</sup>; with a 1:1 cosolvent mixing ratio, rod-like crystals were obtained<sup>[9]</sup>; rectangular plate-like crystals were obtained from NMP/acetonitrile (mixing ratio of 1:4)<sup>[9]</sup>; hexagonal plate-like crystals were obtained from NMP/methanol (mixing ratios of 1:2, 1:3 or 1:4) or NMP/chloroacetone<sup>[9]</sup>

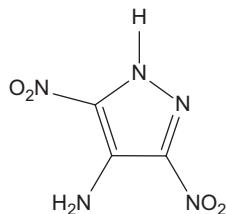
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## 4-Amino-3,5-dinitro-1*H*-pyrazole

Name [German, acronym]: 4-Amino-3,5-dinitropyrazole [4-amino-3,5-dinitropyrazol, LLM-116, ADNP]

Main (potential) use: Inensitive energetic material<sup>[6]</sup>, starting material for many explosives<sup>[6]</sup>

Structural formula:



	<b>LLM-116</b>
Formula	C <sub>3</sub> H <sub>3</sub> N <sub>5</sub> O <sub>4</sub>
Molecular mass [g mol <sup>-1</sup> ]	173.09
Appearance at RT	Yellow crystals of an aggregate of plates <sup>[1]</sup> , golden flat crystals (LLM-116•DMSO solvate) <sup>[1]</sup> , small iridescent yellow plate crystals (LLM-116•H <sub>2</sub> O) <sup>[1]</sup>
IS [J]	DH <sub>50</sub> = 167.5 cm (type 12, 25 mg sample, @ 70 °F, 61% relative humidity (RH)) <sup>[1]</sup> , DH <sub>50</sub> = 165 cm <sup>[2]</sup> , DH <sub>50</sub> = 168 cm <sup>[3]</sup> , DH <sub>50</sub> ≥ 145 cm (2 mg sample in nonhermetic DSC pans, 5 lb mass, nonstandard apparatus, cf. 29 cm for ε-CL-20 and 55 cm for β-HMX using this apparatus) <sup>[4]</sup> , A <sub>d1</sub> = 32%, LL = 1.2 m <sup>[5]</sup> , DH <sub>50</sub> = 177 cm (2.5 kg mass, Bruceton method) <sup>[6]</sup> , DH <sub>50</sub> = 167.5 cm <sup>[7]</sup>
FS [N]	<sup>1</sup> / <sub>10</sub> positive results (BAM, 28.8 kg applied mass, 70 °F ambient T, 67% RH) <sup>[1]</sup> , <sup>0</sup> / <sub>10</sub> @ 36 kg <sup>[3]</sup> , p <sub>fr,LL</sub> = 400 MPa <sup>[5]</sup> , p <sub>fr,50%</sub> = 660 MPa <sup>[5]</sup> , <sup>0</sup> / <sub>10</sub> @ 36 kg (BAM) <sup>[6]</sup>
ESD [J]	No spark sensitivity ( <sup>0</sup> / <sub>10</sub> reaction) to spark (20 kF capacitance, 10.0 kV, 510 Ω resistance, 0.007 in gap, 1.0 J spark energy, 68 °F, 67% RH) <sup>[1]</sup> , no response to spark of 1 J with 510 ohm resistance <sup>[3]</sup> , 0.038 @ 0 <sup>ohm</sup> [6]
N [%]	40.46
Ω(CO <sub>2</sub> ) [%]	-32.4
T <sub>m.p.</sub> [°C]	175–178 (Mel-Temp instrument) <sup>[1]</sup> , 175.70–176.97 (endo, DSC @ 10 °C/min) <sup>[1]</sup> , 160–162 (dec., LLM-116•DMSO solvate) <sup>[1]</sup> , 169–171 (LLM-116•H <sub>2</sub> O) <sup>[1]</sup> , ~180 (with dec.) <sup>[4]</sup> , 173.2 (onset, DSC @ 10 °C/min, hermetic Al pans, N <sub>2</sub> purge) <sup>[4]</sup> , 176 <sup>[6]</sup> , 155 <sup>[8]</sup>

$T_{\text{dec.}}$ [°C]	183.63 (exo, DSC @ 10 °C/min) <sup>[1]</sup> , 178 <sup>[2]</sup> , 180 (onset, DSC) <sup>[3]</sup> , ~180 (melts with dec.) <sup>[4]</sup> , 178.4 (onset, DSC @ 10 °C/min, hermetic Al pans, N <sub>2</sub> purge) <sup>[4]</sup> , 182 (exo peak max, DSC) <sup>[6]</sup>		
$\rho$ [g cm <sup>-3</sup> ]	1.900 (X-ray) <sup>[1]</sup> , 1.608 (crystals, LLM-116•DMSO solvate) <sup>[1]</sup> , 1.90 <sup>[2,4,6,7]</sup> , 1.900 (crystal @ RT) <sup>[3]</sup>		
Heat of formation	−0.2 kcal/mol ( $\Delta H_f^{\circ}$ ) <sup>[3]</sup> , 112.97 kJ/mol ( $\Delta H_f^{\circ}$ , calcd., B3LYP/6-31G(d)) <sup>[7]</sup>		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{\text{ex}} U^{\circ}$ [kJ kg <sup>-1</sup> ]			
$T_{\text{ex}}$ [K]			
$p_{\text{C-J}}$ [kbar]		32.8 GPa (@ 1.900 g cm <sup>-3</sup> , 100% TMD; $\Delta H_f = -0.2$ kcal/mol, calcd., CHEETAH 7.0) <sup>[3]</sup>  23.5 GPa (LLM-175 w/5% PIB @ 95.6% TMD, calcd., CHEETAH 7.0) <sup>[3]</sup>  ~33.3 GPa (@ crystal $\rho$ @ RT, calcd., CHEETAH 7.0) <sup>[4]</sup>  37.15 GPa (@ 1.90 g cm <sup>-3</sup> , $\Delta H_f^{\circ} = 112.97$ kJ/mol, calcd., K-J) <sup>[7]</sup>	
VoD [m s <sup>-1</sup> ]		8,680 (@ 1.900 g cm <sup>-3</sup> , 100% TMD; $\Delta H_f = -0.2$ kcal/mol, calcd., CHEETAH 7.0) <sup>[3]</sup>  7,740 (LLM-175 w/5% PIB @ 95.6% TMD; calcd., CHEETAH 7.0) <sup>[3]</sup>  ~8,510 (@ crystal $\rho$ @ RT, calcd., CHEETAH 7.0) <sup>[4]</sup>  9.00 km/s (@ 1.90 g cm <sup>-3</sup> , $\Delta H_f^{\circ} = 112.97$ kJ/mol, calcd., K-J) <sup>[7]</sup>	
$V_0$ [L kg <sup>-1</sup> ]			

Thermal stability	Stability decreases if impurities of LLM-226 are present <sup>[6]</sup>												
Solubility [g/mL]	Soluble in hot CH <sub>3</sub> CN, DMSO, hot H <sub>2</sub> O, MeOH and EtOH <sup>[1]</sup> , anhydrous LLM-116 recryst. from hot butyl acetate/heptane <sup>[1]</sup> , soluble in water <sup>[6]</sup> , soluble in ethyl acetate <sup>[6]</sup> , soluble in toluene, Et <sub>2</sub> O, benzene/Et <sub>2</sub> O, benzene/acetic acid, 1,2-dichloroethane <sup>[6]</sup>												
CRT (chemical reactivity test)	0.002 cc/0.25 g gas produced (0.25 g sample @ 80 °C) <sup>[1]</sup> , rapid dec. @ 120 °C <sup>[1]</sup> , 0.6 cc/g @ 80 °C <sup>[3]</sup>												
DAX experiments	Data from <sup>[3]</sup> : <table border="1"> <thead> <tr> <th>Sample</th> <th>Density/% TMD</th> <th>VoD (km/s)</th> <th>CJ jump-off</th> <th>JWL CJ</th> <th>DAX E<sub>3</sub> (kJ/cc)</th> </tr> </thead> <tbody> <tr> <td>ADNP 95%</td> <td>1.722/95.6</td> <td>8.130</td> <td>28.9</td> <td>28.9</td> <td>4.84</td> </tr> </tbody> </table>	Sample	Density/% TMD	VoD (km/s)	CJ jump-off	JWL CJ	DAX E <sub>3</sub> (kJ/cc)	ADNP 95%	1.722/95.6	8.130	28.9	28.9	4.84
Sample	Density/% TMD	VoD (km/s)	CJ jump-off	JWL CJ	DAX E <sub>3</sub> (kJ/cc)								
ADNP 95%	1.722/95.6	8.130	28.9	28.9	4.84								
pH	pK <sub>BH+</sub> = -5.43 <sup>[8]</sup>												

	LLM-116 <sup>[1]</sup>	LLM-116•DMSO <sup>[1]</sup>	LLM-116•H <sub>2</sub> O <sup>[1]</sup>
Chemical formula	C <sub>3</sub> H <sub>3</sub> N <sub>5</sub> O <sub>4</sub>	C <sub>5</sub> H <sub>9</sub> N <sub>5</sub> O <sub>5</sub> S	C <sub>3</sub> H <sub>5</sub> N <sub>5</sub> O <sub>5</sub>
Molecular weight [g mol <sup>-1</sup> ]	173.10	251.23	191.12
Crystal system	Orthorhombic	Monoclinic	Orthorhombic
Space group	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	P2 <sub>1</sub> /c	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>
a [Å]	4.7257(5)	10.8977(8)	4.658(4)
b [Å]	4.7312(6)	14.1398(11)	5.010(4)
c [Å]	27.063(4)	6.7767(6)	30.54(2)
α [°]	90	90	90
β [°]	90	96.453(6)	90
γ [°]	90	90	90
V [Å <sup>3</sup> ]	605.07(13)	1,037.61(14)	712.8(9)
Z	4	4	4
ρ <sub>calc</sub> [g cm <sup>-3</sup> ]	1.900 (@ 21 °C)	1.608	1.781
T [K]	294	295	295

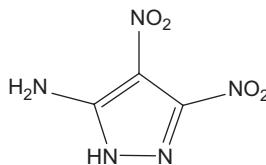
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- [6] M.-X. Zhang, P. F. Pagoria, G. H. Imler, D. Parrish, *J. Heterocyclic Chem.*, **2019**, *56*, 781–787.
- [7] Z. Guozheng, L. Ming, *J. Energet. Mater.*, **2013**, *31*, 60–71.
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## 5-Amino-3,4-dinitropyrazole

Name [German, acronym]: 5-Amino-3,4-dinitropyrazole, [5-amino-3,4-dinitropyrazol, 5-ADP]

Main (potential) use: Possible future energetic component<sup>[1]</sup>

Structural formula:



	<b>5-ADP</b>
Formula	$\text{C}_3\text{H}_3\text{N}_5\text{O}_4$
Molecular mass [g mol <sup>-1</sup> ]	173.09
Appearance at RT	Crystallites composed of flakes of 15 $\mu\text{m}$ lateral size and nanosized thickness <sup>[1]</sup>
IS [J]	$H_{50\%} = 23 \pm 2$ (BAM, STANAG 4489) <sup>[1]</sup>
FS [N]	Insensitive (BAM) <sup>[1]</sup> , only 40% explosions @ max load of 360 N (BAM) <sup>[1]</sup>
ESD [J]	-32
N [%]	40.45
$\Omega(\text{CO}_2)$ [%]	-32.4
$T_{\text{m.p.}}$ [°C]	195 (DSC @ 5 K/min, closed alumina pan with pierced lid) <sup>[1]</sup> , immediate dec. on melting (TGA @ 10 K/min, sharp exo peak and 40% mass loss, liquid-state dec., closed alumina pan with pierced lid) <sup>[1]</sup> , at lower heating rates, solid-state dec. occurs @ $T < \text{mpt.}$ (DSC @ 0.5 K/min, closed alumina pan with pierced lid) <sup>[1]</sup> , 197–199 (with dec., recryst. sample from water) <sup>[2]</sup>
$T_{\text{phase transition}}$ [°C]	No features observed in DSC before melting point (DSC @ 5 K/min, closed alumina pan with pierced lid) <sup>[1]</sup>
$T_{\text{dec.}}$ [°C]	198 (extrapolated onset $T$ , DSC @ 5 K/min, closed alumina pan with pierced lid) <sup>[1]</sup> , immediate dec. on melting (TGA @ 10 K/min, sharp exo peak and 40% mass loss, liquid-state dec.) <sup>[1]</sup> , at lower heating rates, solid-state dec. occurs @ $T < \text{mpt.}$ (DSC @ 0.5 K/min, closed alumina pan with pierced lid) <sup>[1]</sup> , 201.3 (TG @ 5 K/min, 46% mass loss) <sup>[1]</sup> , 198.5 (DTG @ 5 K/min, 21.35% mass loss) <sup>[1]</sup> , 202.2 (DSC @ 5 K/min, exo peak max) <sup>[1]</sup> , 197–199 (melts with dec.) <sup>[2]</sup>
$\rho$ [g cm <sup>-3</sup> ]	1.87 <sup>[1]</sup>
Heat of formation	60 kJ/mol (exptl.) <sup>[1]</sup>

	Calcd. (EXPLO5 6.03)	Lit. values		Exptl.																																																									
$-\Delta_{\text{ex}}U^{\circ}$ [kJ kg <sup>-1</sup> ]																																																													
$T_{\text{ex}}$ [K]																																																													
$p_{\text{CJ}}$ [kbar]		33.7 GPa (@ 1.87 g cm <sup>-3</sup> , calcd., BKW) <sup>[1]</sup>																																																											
		31.6 GPa (@ 1.87 g cm <sup>-3</sup> , calcd., Kamlet) <sup>[1]</sup>																																																											
VoD [m s <sup>-1</sup> ]		8,550 (@ 1.87 g cm <sup>-3</sup> , calcd., BKW) <sup>[1]</sup>																																																											
		8,350 (@ 1.87 g cm <sup>-3</sup> , calcd., Kamlet) <sup>[1]</sup>																																																											
$V_0$ [L kg <sup>-1</sup> ]																																																													
Thermal stability [°C]	173 (5-ADP/active binder mix, ARC (accelerating rate calorimeter)) <sup>[1]</sup>																																																												
Burn rate [mm/s]	$U_b = 14.3 \text{ mm s}^{-1}$ @ 7 MPa, pressure exponent = $0.51 \pm 0.04$ (constant pressure bomb, $V = 1.5 \text{ L}$ , 2–12 MPa pressure range, 8 mm inside diameter pressed cylinders, coated on lateral surface with epoxy glue) <sup>[1]</sup>																																																												
Solubility [g/mL]	Recryst. from water <sup>[2]</sup>																																																												
Compatibility	<p>Good compatibility with common energetic materials, for example, TNT, RDX, AP<sup>[1]</sup></p> <p>Data from<sup>[1]</sup> (A = compatible or good compatibility, B = slightly sensitized or fair compatibility, C = sensitized or poor compatibility, D = hazardous or bad compatibility):</p> <table border="1"> <thead> <tr> <th>Additive</th> <th>DSC</th> <th><math>\Delta T_p</math> (°C)</th> <th>Rating</th> <th><math>T_p</math> (°C)</th> <th><math>\Delta T_p</math> (°C)</th> <th>Rating</th> </tr> </thead> <tbody> <tr> <td>Al</td> <td>204</td> <td>2</td> <td>A</td> <td>203</td> <td>-2</td> <td>A</td> </tr> <tr> <td>TNT</td> <td>209</td> <td>-7</td> <td>A</td> <td>208</td> <td>-7</td> <td>A</td> </tr> <tr> <td>HMX</td> <td>198</td> <td>4</td> <td>B</td> <td>197</td> <td>4</td> <td>B</td> </tr> <tr> <td>CL-20</td> <td>199</td> <td>3</td> <td>B</td> <td>198</td> <td>2</td> <td>A</td> </tr> <tr> <td>AP</td> <td>213</td> <td>-11</td> <td>A</td> <td>212</td> <td>-11</td> <td>A</td> </tr> <tr> <td>Active binder</td> <td>178</td> <td>7</td> <td>C</td> <td>177</td> <td>5</td> <td>B</td> </tr> <tr> <td>Inert binder</td> <td>226</td> <td>-24</td> <td>A</td> <td>224</td> <td>-23</td> <td>A</td> </tr> </tbody> </table>					Additive	DSC	$\Delta T_p$ (°C)	Rating	$T_p$ (°C)	$\Delta T_p$ (°C)	Rating	Al	204	2	A	203	-2	A	TNT	209	-7	A	208	-7	A	HMX	198	4	B	197	4	B	CL-20	199	3	B	198	2	A	AP	213	-11	A	212	-11	A	Active binder	178	7	C	177	5	B	Inert binder	226	-24	A	224	-23	A
Additive	DSC	$\Delta T_p$ (°C)	Rating	$T_p$ (°C)	$\Delta T_p$ (°C)	Rating																																																							
Al	204	2	A	203	-2	A																																																							
TNT	209	-7	A	208	-7	A																																																							
HMX	198	4	B	197	4	B																																																							
CL-20	199	3	B	198	2	A																																																							
AP	213	-11	A	212	-11	A																																																							
Active binder	178	7	C	177	5	B																																																							
Inert binder	226	-24	A	224	-23	A																																																							
$\text{p}K_a$	6.34 (@ 20 °C in water, spectrophotometrically) <sup>[2]</sup> , $\text{p}K_{\text{BH}^+} = -7.12$ (@ 20 °C in water, spectrophotometrically) <sup>[2]</sup>																																																												

	<b>5-ADP<sup>[1]</sup></b>	<b>5-ADP<sup>[1]</sup></b>
Chemical formula	C <sub>3</sub> H <sub>3</sub> N <sub>5</sub> O <sub>4</sub>	C <sub>3</sub> H <sub>3</sub> N <sub>5</sub> O <sub>4</sub>
Molecular weight [g mol <sup>-1</sup> ]	173.02	173.02
Crystal system	Monoclinic	Monoclinic
Space group	P2 <sub>1</sub> /c (no. 14)	
<i>a</i> [Å]	7.2109(9)	7.2132(3)
<i>b</i> [Å]	12.4309(16)	12.4258(5)
<i>c</i> [Å]	7.1649(9)	7.1589(3)
$\alpha$ [°]	90	90
$\beta$ [°]	106.795(3)	106.814(2)
$\gamma$ [°]	90	90
<i>V</i> [Å <sup>3</sup> ]	614.85(14)	614.30(4)
<i>Z</i>	4	
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.8699(4)	
<i>T</i> [K]	RT	
	X-ray powder diffraction, sample showed 99.5 wt.% purity with 0.5% crystalline impurities	Calcd. X-ray diffraction

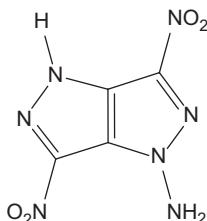
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## 1-Amino-3,6-dinitropyrazolo[4,3-*c*]pyrazole

Name [German, acronym]: 1-Amino-3,6-dinitropyrazolo[4,3-*c*]pyrazole,  
 [1-amino-3,6-dinitropyrazolo[4,3-*c*]pyrazol]

Main (potential) use: high explosive

Structural formula:



	1-Amino-3,6-dinitropyrazolo[4,3- <i>c</i> ]pyrazole		
Formula	$C_4H_3N_7O_4$		
Molecular mass [g mol <sup>-1</sup> ]	213.11		
Appearance at RT	Brown solid <sup>[1]</sup>		
IS [J]	14 (BAM) <sup>[1]</sup>		
FS [N]	280 (BAM) <sup>[1]</sup>		
N [%]	46.01		
$\Omega(CO_2)$ [%]	−41.3		
$T_{dec.}$ [°C]	178 <sup>[1]</sup>		
$\rho$ [g cm <sup>−3</sup> ]	1.74 (gas pycnometer) <sup>[1]</sup>		
Heat of formation			
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{ex}U^\circ$ [kJ kg <sup>−1</sup> ]			
$T_{ex}$ [K]			
$p_{C-J}$ [kbar]		27.9 GPa (@ 1.74 g cm <sup>−3</sup> , calcd., K-J) <sup>[1]</sup>	
VoD [m s <sup>−1</sup> ]		7,934 (@ 1.74 g cm <sup>−3</sup> , calcd., K-J) <sup>[1]</sup>	
$V_0$ [L kg <sup>−1</sup> ]			

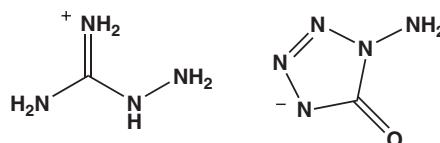
[1] Y. Li, Y. Shu, B. Wang, S. Zhang, L. Zhai, *RSC Adv.*, **2016**, *6*, 84,760–84,768.

## Aminoguanidinium 1-aminotetrazol-5-oneate

Name [German, acronym]: Aminoguanidinium 1-aminotetrazol-5-oneate [ATO•AG]

Main (potential) use: Secondary (high) explosive

Structural formula:



	ATO • AG
Formula	C <sub>2</sub> H <sub>9</sub> N <sub>9</sub> O
Molecular mass [g mol <sup>-1</sup> ]	175.18
Appearance at RT	Yellow powder <sup>[1]</sup>
IS [J]	>40 <sup>[1]</sup>
N [%]	72.0
Ω(CO) [%]	-50.29
T <sub>m.p.</sub> [°C]	197.5 (DSC-TG @ 10 °C/min) <sup>[1]</sup>
T <sub>dec.</sub> [°C]	220.6 (DSC @ 5 °C/min) <sup>[1]</sup>
ρ [g cm <sup>-3</sup> ]	1.597 (cryst., @ 296 K) <sup>[1]</sup>
Heat of formation	420.51 kJ/mol (Δ <sub>f</sub> H <sup>o</sup> , calcd.) <sup>[1]</sup> , 2,402.9 kJ kg <sup>-1</sup> (Δ <sub>f</sub> H <sup>o</sup> , calcd.) <sup>[1]</sup>
Calcd. (K-J)	Exptl.
-Δ <sub>ex</sub> U <sup>o</sup> [kJ kg <sup>-1</sup> ]	
T <sub>ex</sub> [K]	
p <sub>CJ</sub> [GPa]	26.7 <sup>[1]</sup>
V <sub>oD</sub> [m s <sup>-1</sup> ]	8,160 <sup>[1]</sup>
V <sub>0</sub> [L kg <sup>-1</sup> ]	

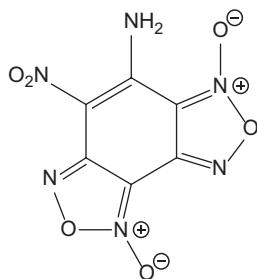
	<b>ATO•AG<sup>[1]</sup></b>
Chemical formula	C <sub>2</sub> H <sub>9</sub> N <sub>9</sub> O
Molecular weight [g mol <sup>-1</sup> ]	175.18
Crystal system	Monoclinic
Space group	P2 <sub>1</sub> /n (14)
<i>a</i> [Å]	8.5361(4)
<i>b</i> [Å]	6.5988(3)
<i>c</i> [Å]	13.2935(7)
$\alpha$ [°]	90
$\beta$ [°]	103.3740(10)
$\gamma$ [°]	90
<i>V</i> [Å <sup>3</sup> ]	728.49(6)
<i>Z</i>	4
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.597
<i>T</i> [K]	296

[1] X. Yin, J.-T. Wu, X. Jin, C.-X. Xu, P. He, T. Li, K. Wang, J. Qin, J.-G. Zhang, *RSC Adv.*, **2015**, *5*, 60,005–60,014.

## Aminonitrobenzodifuroxan

Name [German, acronym]: 4-Amino5-nitrobenzo-4-[1,2-c:3,4-c']bis[1,2,5]oxadiazole-3,8-dioxide, 8-amino-7-nitrobenzobisfuroxan  
[aminonitrobenzodifuroxan, CL-18]

Main (potential) use: Possible new insensitive high explosive<sup>[1]</sup>  
Structural formula:



	CL-18
Formula	C <sub>6</sub> H <sub>2</sub> N <sub>6</sub> O <sub>6</sub>
Molecular mass [g mol <sup>-1</sup> ]	254.12
Appearance at RT	Yellow crystalline solid <sup>[2]</sup>
IS [J]	DH <sub>50</sub> = 56 cm <sup>[1,2]</sup> , H <sub>50</sub> = 33 cm (NWC's impact tester) <sup>[2]</sup> , H <sub>50%</sub> = 56 cm (2.5 kg mass, type 12 tool, 35 mg sample in conical pile, 1 in <sup>2</sup> garnet paper) <sup>[3]</sup>
FS [N]	10/10 NF @ 794 lb <sup>[2]</sup>
ESD [J]	14/20 NF @ 0.25 <sup>[2]</sup>
N [%]	33.07
Ω(CO <sub>2</sub> ) [%]	-44.07
T <sub>m.p.</sub> [°C]	205 (Kofler hot-stage apparatus) <sup>[1,2]</sup> , 205–210 (crude product from acetic acid preparation, Kofler hot-stage apparatus) <sup>[2]</sup> , 201–204 (acetic acid prep., product recryst. from boiling acetic acid, Kofler hot-stage apparatus) <sup>[2]</sup> , 185–200 (crude product from dichloroethane preparation, Kofler hot-stage apparatus) <sup>[2]</sup>
T <sub>phase transition</sub> [°C]	186–195 <sup>[2]</sup>
T <sub>dec.</sub> [°C]	
ρ [g cm <sup>-3</sup> ]	1.93 <sup>[1–3]</sup>
Heat of formation	

	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{\text{ex}} U^{\circ} [\text{kJ kg}^{-1}]$			
$T_{\text{ex}} [\text{K}]$			
$p_{\text{CJ}} [\text{kbar}]$		312 (@ 1.98 g cm <sup>-3</sup> , calcd.) <sup>[3]</sup>	
VoD [m s <sup>-1</sup> ]		8,370 (@ 1.93 g cm <sup>-3</sup> , calcd.) <sup>[2]</sup>  8,230 (@ 1.98 g cm <sup>-3</sup> , calcd.) <sup>[3]</sup>	
$V_0 [\text{L kg}^{-1}]$			

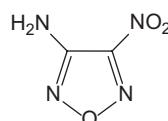
- [1] L. Türker, S. Varis, *A Review of Polycyclic Aromatic Energetic Materials*, in *Polycyclic Aromatic Compounds*, **2009**, 29, 228–266.
- [2] S. L. Christian, A. P. Chafin, A. T. Nielsen, R. L. Atkins, W. P. Norris, R. A. Hollins, *Synthesis of Aminonitrobenzodifuroxan*, US Patent 5,149,818, September 22nd **1992**.
- [3] W. S. Wilson, D. E. Bliss, S. L. Christian, D. J. Knight, *Explosive Properties of Polynitroaromatics*, NWC TP 7073, Naval Weapons Center, China Lake, USA, April **1990**.

## 3-Amino-4-nitrofurazan

Name [German, acronym]: Aminonitrofuran [ANF]

Main (potential) use: secondary explosive

Structural formula:



	<b>ANF</b>		
Formula	C <sub>2</sub> H <sub>2</sub> N <sub>4</sub> O <sub>3</sub>		
Molecular mass [g mol <sup>-1</sup> ]	130.06		
Appearance at RT	Yellow crystals <sup>[2]</sup>		
IS [J]	10 (1/6, BAM) <sup>[3]</sup>		
FS [N]	360 (1/6, BAM) <sup>[3]</sup>		
ESD [J]	0.3 (OZM apparatus) <sup>[3]</sup>		
N [%]	43.08		
Ω(CO <sub>2</sub> ) [%]	-24.60		
T <sub>m.p.</sub> [°C]	122 <sup>[1]</sup> , 119–120 <sup>[2]</sup> , 121 (DTA @ 5 °C/min) <sup>[3]</sup>		
T <sub>dec.</sub> [°C]	143 (DTA @ 5 °C/min) <sup>[3]</sup>		
ρ [g cm <sup>-3</sup> ]	1.808 (X-ray, @ 298 K) <sup>[3]</sup>		
Heat of formation	156.7 kJ/mol (Δ <sub>f</sub> H°, calcd., CBS-4M) <sup>[3]</sup> , 1,290.7 kJ/kg (Δ <sub>f</sub> U°, calcd., CBS-4M) <sup>[3]</sup>		
	Calcd. (EXPLO5 6.02)	Lit. values	Exptl.
-Δ <sub>ex</sub> U° [kJ kg <sup>-1</sup> ]	5,712 <sup>[3]</sup>		
T <sub>ex</sub> [K]	4,015 <sup>[3]</sup>		
p <sub>C-J</sub> [kbar]	373 <sup>[3]</sup>		
VoD [m s <sup>-1</sup> ]	8,769 (@ 1.808 g cm <sup>-3</sup> ) <sup>[3]</sup>		
V <sub>0</sub> [L kg <sup>-1</sup> ]	743 <sup>[3]</sup>		

	Aminonitrofurazan <sup>[1]</sup>	Aminonitrofurazan <sup>[3]</sup>
Chemical formula	C <sub>2</sub> H <sub>2</sub> N <sub>4</sub> O <sub>3</sub>	C <sub>2</sub> H <sub>2</sub> N <sub>4</sub> O <sub>3</sub>
Molecular weight [g mol <sup>-1</sup> ]	130.06	130.06
Crystal system	Orthorhombic	Orthorhombic
Space group	Pna2 <sub>1</sub>	Pna2 <sub>1</sub>
a [Å]	14.864(16)	
b [Å]	5.385(6)	
c [Å]	11.630(15)	
α [°]	90	90
β [°]	90	90
γ [°]	90	90
V [Å <sup>3</sup> ]	931(3)	938.26
Z	8	8
ρ <sub>calc</sub> [g cm <sup>-3</sup> ]	1.86	1.842 (@ 173 K) 1.84 (@ 153 K)
T [K]	-120 °C	173

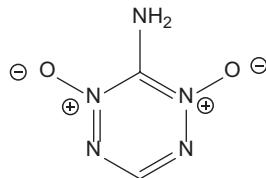
- [1] A. S. Batsanov, Y. T. Struchkov, *J. Struct. Chem.*, **1985**, *26*, 52–56.
- [2] B. J. Schiren, *Synthesis of Energetic Furazan Derivatives*, Master Thesis, Indiana University of Pennsylvania, May 2012.
- [3] T. M. Klapötke, P. C. Schmid, J. Stierstorfer, *Crystals*, **2015**, *5*, 418–432.

### 3-Amino-6-nitro-1,2,4,5-tetrazino-2,4-dioxide

Name [German, acronym]: 3-Amino-6-nitro-1,2,4,5-tetrazino-2,4-dioxide  
 [3-amino-6-nitro-1,2,4,5-tetrazino-2,4-dioxid]

Main (potential) use: secondary explosive

Structural formula:



	3-Amino-6-nitro-1,2,4,5-tetrazino-2,4-dioxide		
Formula	$C_2H_3N_5O_2$		
Molecular mass [g mol <sup>-1</sup> ]	129.08		
Appearance at RT			
IS [J]			
FS [N]			
ESD [J]			
N [%]	54.26		
$\Omega(CO_2)$ [%]	-43.4		
$T_{m.p.}$ [°C]			
$T_{\text{phase transition}}$ [°C]			
$T_{\text{dec.}}$ [°C]			
$\rho$ [g cm <sup>-3</sup> ]	1.919 (X-ray) <sup>[1]</sup>		
Heat of formation			
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^\theta$ [kJ kg <sup>-1</sup> ]			
$T_{\text{ex}}$ [K]			
$p_{\text{C-J}}$ [kbar]			
VoD [m s <sup>-1</sup> ]			
$V_0$ [L kg <sup>-1</sup> ]			

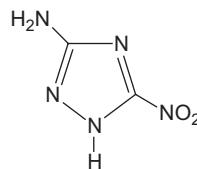
[1] D. E. Chavez, M A. Hiskey, *J. Energet. Mater.*, **1999**, *17*, 357–377.

### 3-Amino-5-nitro-1,2,4-triazole

Name [German, acronym]: 5-Amino-3-nitro-1*H*-1,2,4-triazole, [3-amino-5-nitro-1,2,4-triazol, ANTA]

Main (potential) use: Possible use in propellant/explosive formulations in which thermal stability and insensitivity are important<sup>[1,16]</sup>, insensitive energetic material<sup>[2,9]</sup>, low-energy insensitive explosive<sup>[5]</sup>, insensitive high explosive with possible potential to replace NTO<sup>[6]</sup>, under evaluation as possible IHE for nuclear weapons<sup>[6]</sup>, useful intermediate in preparation of other energetic materials<sup>[9]</sup>

Structural formula:



	<b>ANTA</b>
Formula	C <sub>2</sub> H <sub>3</sub> N <sub>5</sub> O <sub>2</sub>
Molecular mass [g mol <sup>-1</sup> ]	129.08
Appearance at RT	Yellow crystalline solid <sup>[5]</sup> , pale straw-colored crystals (ANTA•H <sub>2</sub> O) <sup>[11]</sup>
IS [J]	>170 cm <sup>[1,16]</sup> , >177 cm (too low to be determined with 177 cm height limit, i.e., >177 cm, 2.5 kg mass, type 12 tool, 35 mg pressed sample) <sup>[5]</sup> , >170 cm (2 kg mass, Bruceton method) <sup>[6]</sup> , 100 <sup>[7]</sup> , >320 cm (type 12, similar to that of TATB) <sup>[9]</sup>
FS [N]	16.8 kg (1/10, Julius-Peters) <sup>[5]</sup> , insensitive up to 36 kg (Julius-Peters) <sup>[6]</sup>
ESD [J]	No reaction (10 tries @ 1 J with 510 Ω in-line resistance) <sup>[5]</sup> , >1.0 (3 mil foil) <sup>[9]</sup>
N [%]	54.26
Ω(CO <sub>2</sub> ) [%]	-43.4
T <sub>m.p.</sub> [°C]	240 <sup>[1,16]</sup> , 238 <sup>[2,6]</sup> , 238–241 (crystals) <sup>[5]</sup> , 249 (endo, DTA) <sup>[6]</sup> , 240 (endo, DSC @ 10 °C/min) <sup>[6]</sup> , 244 <sup>[9]</sup>
T <sub>phase transition</sub> [°C]	Two polymorphs: α (monoclinic) and β- (monoclinic, obtained by recryst. from 2-butanone), <sup>[5]</sup> Two polymorphs: α from recryst. from CHCl <sub>3</sub> /EtOH soln. (monoclinic, C2/c) and β from recryst. from 1-butanol (monoclinic, P2 <sub>1</sub> /n) <sup>[10]</sup>

$T_{\text{dec.}} [^{\circ}\text{C}]$	227 (onset), 243 (peak max) (DSC @ 10 °C/min) <sup>[5]</sup> , 243–277 (first stage, 38% weight loss, TG) <sup>[6]</sup> , 277–563 (second stage, slow, 51% weight loss, TG) <sup>[6]</sup> , 260 (exo, first stage dec., DTA) <sup>[6]</sup> , 245 (exo peak max., DSC @ 10 °C/min) <sup>[6]</sup> , 214 (exo peak max., DSC @ 5 °C/min) <sup>[6]</sup> , 250 (exo peak max., DSC @ 15 °C/min) <sup>[6]</sup> , 253 (exo peak max., DSC @ 20 °C/min) <sup>[6]</sup> , 256 (exo peak max., DSC @ 25 °C/min) <sup>[6]</sup> , 210–240 (DSC, TGA two or possibly three overlapping stages of dec. occur) <sup>[8]</sup>		
$\rho [\text{g cm}^{-3}]$	1.82 <sup>[1,6,7,16]</sup> , 1.819 <sup>[2]</sup> , 1.82 (crystal) <sup>[9,13]</sup> , 1.811 (calcd., EDPHT 2.0) <sup>[13]</sup> , 1.745 (calcd., Ammon) <sup>[13]</sup>		
Heat of formation	61 kcal/mol ( $\Delta H_f$ ) <sup>[2]</sup> , $88 \pm 10$ kJ/mol ( $\Delta H_f^\ominus$ ) <sup>[3]</sup> , $61.1 \pm 4$ kJ/mol (calcd. from heat of combustion value) <sup>[5]</sup> , 188.7 kJ/mol ( $\Delta H_f(\text{g})$ ) <sup>[7]</sup> , 77.1 kJ/mol ( $\Delta H_f(\text{s})$ ) <sup>[7]</sup> , 87.8 kJ/mol ( $\Delta H_f^{\text{exptl}}(\text{s})$ ) <sup>[7]</sup> , $21.0 \pm 2.5$ kcal/mol <sup>[9]</sup>		
Heat of combustion	$-9.891 \pm 0.008$ kJ/g (exptl., calorimeter) <sup>[5]</sup>		
	Calcd. (EXPLO5 5.05) <sup>[7]</sup>	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^\ominus [\text{kJ kg}^{-1}]$	4,194 (@ 1.791 g cm <sup>-3</sup> , $\Delta H_f = 77.1$ kJ mol <sup>-1</sup> ) <sup>[7]</sup>		
$T_{\text{ex}} [\text{K}]$	3,227 (@ 1.791 g cm <sup>-3</sup> , $\Delta H_f = 77.1$ kJ mol <sup>-1</sup> ) <sup>[7]</sup>		
$p_{\text{C-J}} [\text{kbar}]$	276 (@ 1.791 g cm <sup>-3</sup> , $\Delta H_f = 77.1$ kJ mol <sup>-1</sup> ) <sup>[7]</sup>		
VoD [m s <sup>-1</sup> ]	8,181 (@ 1.791 g cm <sup>-3</sup> , $\Delta H_f = 77.1$ kJ mol <sup>-1</sup> ) <sup>[7]</sup>	8,460 (@ 1.82 g cm <sup>-3</sup> , calcd.) <sup>[1]</sup>	
$V_0 [\text{L kg}^{-1}]$	736 (@ 1.791 g cm <sup>-3</sup> , $\Delta H_f = 77.1$ kJ mol <sup>-1</sup> ) <sup>[7]</sup>		
5 s explosion $T$ [°C] Deflagration $T$ [°C]	258 <sup>[6]</sup>		
Vacuum stability test [cm <sup>3</sup> /h]	0.3 mL/h/48 h @ 120 °C <sup>[9]</sup> , 0.3104 mL/5 g @ 94 °C for 48 h <sup>[12]</sup>		
Solubility [g/mL]	Recryst. from H <sub>2</sub> O, EtOH <sup>[5]</sup> , soluble in DMSO <sup>[9]</sup>		
CRT	0.24 cm <sup>3</sup> /g (@ 120 °C for 22 h under 1 atm He) <sup>[5]</sup>		
$\Delta E_{\text{dec}}$ [J/g]	1,680 <sup>[6]</sup>		
$\Delta H_{\text{subl}}$ [J/g]	111.6 <sup>[7]</sup>		
$pK_a$	7.05 (ring nitrogen H atom) <sup>[10]</sup>		

	<b>ANTA<sup>[4]</sup></b>	<b>ANTA•H<sub>2</sub>O<sup>[11]</sup></b>
Chemical formula	C <sub>2</sub> H <sub>3</sub> N <sub>5</sub> O <sub>2</sub>	C <sub>2</sub> H <sub>3</sub> N <sub>5</sub> O <sub>2</sub> •H <sub>2</sub> O
Molecular weight [g mol <sup>-1</sup> ]	129.1	147.09
Crystal system	Monoclinic	Monoclinic
Space group	C2/c	P2 <sub>1</sub> /c
<i>a</i> [Å]	14.199(4)	11.129(3)
<i>b</i> [Å]	4.844(1)	15.227(3)
<i>c</i> [Å]	14.258(4)	7.130(2)
$\alpha$ [°]	90	90
$\beta$ [°]	105.98(1)	101.29(2)
$\gamma$ [°]	90	90
<i>V</i> [Å <sup>3</sup> ]	942.7(4)	1,184.88
<i>Z</i>	8	8
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.819	1.649
<i>T</i> [K]	RT	RT
	Yellow crystals from EtOH/ CHCl <sub>3</sub> mixture	Hydrate of ANTA

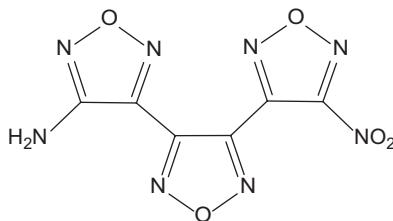
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- [12] A. K. Sikder, G. M. Bhokare, D. B. Sarwade, J. P. Agrawal, *Propellants, Explosives, Pyrotechnics*, **2001**, *26*, 63–68.
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### 3-(4-Amino-1,2,5-oxadiazol-3-yl)-4-(4-nitro-1,2,5-oxadiazol-3-yl)-1,2,5-oxadiazole

Name [German, acronym]: 3-(4-Nitro-1,2,5-oxadiazol-3-yl)-4-(4-amino-1,2,5-oxadiazol-3-yl)-1,2,5-oxadiazole, 4-amino-4"-nitro[3,3',4',3"]-trifurazans [ANFF-1, LLM-175, ANTF]

Main (potential) use: Possible future melt-castable secondary explosive<sup>[1]</sup>, possible future secondary explosive, oxidizer and melt-castable explosive<sup>[2]</sup>, possible new melt-castable explosive replacement for TNT<sup>[4]</sup>

Structural formula:



	<b>ANFF-1</b>
Formula	C <sub>6</sub> H <sub>2</sub> N <sub>8</sub> O <sub>5</sub>
Molecular mass [g mol <sup>-1</sup> ]	266.13
Appearance at RT	White powder <sup>[2]</sup> , white needles (recryst. from CHCl <sub>3</sub> ) <sup>[2]</sup> , white solid <sup>[3]</sup>
IS [J]	43.4 <sup>[1]</sup> , >177 cm (2.5 kg mass, 0.64 × 0.57 × 0.43 mm <sup>3</sup> crystals) <sup>[2]</sup> , DH <sub>50</sub> ≥ 177 cm <sup>[3]</sup>
FS [N]	>353 <sup>[1]</sup> , 0/ <sub>10</sub> @ 36 kg (BAM, 0.64 × 0.57 × 0.43 mm <sup>3</sup> crystals) <sup>[2]</sup> , 1/ <sub>10</sub> @ 24 kg <sup>[3]</sup>
ESD [J]	No response to spark of 1 J with 510 ohm resistance <sup>[3]</sup>
N [%]	42.11
Ω(CO <sub>2</sub> ) [%]	-27
T <sub>m.p.</sub> [°C]	100 <sup>[1,4]</sup> , 103.1 (endo peak max, DSC @ 10 °C/min) <sup>[4]</sup>
T <sub>dec.</sub> [°C]	234 (onset, DSC) <sup>[3]</sup> , 240.9 (exo peak max, DSC @ 10 °C/min) <sup>[4]</sup>
ρ [g cm <sup>-3</sup> ]	1.782 <sup>[1,2]</sup> , 1.782 (crystal density @ 293 K) <sup>[3]</sup>
Heat of formation	

	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{\text{ex}} U^{\circ} [\text{kJ kg}^{-1}]$			
$T_{\text{ex}} [\text{K}]$		4,286 (@ 1.782 g cm <sup>-3</sup> , $\Delta H_f = 688.0 \text{ kJ/mol}$ , calcd., JAGUAR) <sup>[5]</sup>	
$p_{\text{C-J}} [\text{kbar}]$		<p>27.0 GPa (@ 1.782 g cm<sup>-3</sup>, 100% TMD, <math>\Delta H_f = 159.5 \text{ kcal/mol}</math>, calcd., CHEETAH 7.0)<sup>[3]</sup></p> <p>25.1 GPa (LLM-175 w/5% PIB @ 97.0% TMD, <math>\Delta H_f = 159.5 \text{ kcal/mol}</math>, calcd., CHEETAH 7.0)<sup>[3]</sup></p> <p>29.64 GPa (@ 1.782 g cm<sup>-3</sup>, calcd., K-J)<sup>[4]</sup></p> <p>30.8 GPa (@ 1.782 g cm<sup>-3</sup>, <math>\Delta H_f = 688.0 \text{ kJ/mol}</math>, calcd., JAGUAR)<sup>[5]</sup></p>	
VoD [m s <sup>-1</sup> ]		<p>8,100 (@ 1.782 g cm<sup>-3</sup>, 100% TMD, <math>\Delta H_f = 159.5 \text{ kcal/mol}</math>, calcd., CHEETAH 7.0)<sup>[3]</sup></p> <p>7,410 (LLM-175 w/5% PIB @ 97.0% TMD, <math>\Delta H_f = 159.5 \text{ kcal/mol}</math>, calcd., CHEETAH 7.0)<sup>[3]</sup></p> <p>8,200 (@ 1.782 g cm<sup>-3</sup>, calcd., K-J)<sup>[4]</sup></p> <p>8,220 (@ 1.782 g cm<sup>-3</sup>, <math>\Delta H_f = 688.0 \text{ kJ/mol}</math>, calcd., JAGUAR)<sup>[5]</sup></p>	
$V_0 [\text{L kg}^{-1}]$			
Solubility [g/mL]	Recryst. from CHCl <sub>3</sub> <sup>[2]</sup>		
CRT	0.9 cc/g @ 120 °C <sup>[3]</sup>		

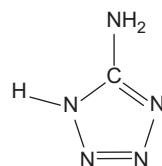
DAX experiments	Summary of results from DAX experiments and JWL modeling for LLM-175 formulation, pressings <sup>[3]</sup> : LLM-175, 95%, $\rho = 1.650 \text{ g/cm}^3$ (97.0% TMD), VoD = 7.729 km/s, C-J jump off = 31.4, JWL CJ = 24.5, DAX $E_3 = 5.01 \text{ kJ/cc}$ <sup>[3]</sup>
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## 5-Aminotetrazole

- Name [German, acronym]: Aminotetrazole, 1*H*-tetrazol-5-amine, 5-amino-1*H*-tetrazole [aminotetrazol, 5-ATZ, 5-AT]
- Main (potential) use: Starting material for synthesis of various energetic materials, gas-generating agent for air bag inflators,<sup>[4]</sup> in solid propellants with KNO<sub>3</sub>, Sr(NO<sub>3</sub>)<sub>2</sub> and strontium nitrate oxidizers<sup>[8]</sup>, thermally stable, nonexplosive prospective candidate for gas generation at high temperatures<sup>[10]</sup>, gas-generating agent and solid propellant<sup>[14]</sup>, burn rate modifier, fire suppressor and environmentally friendly gas-generating agent<sup>[15]</sup>, for synthesis of tetrazole compounds<sup>[17]</sup>

Structural formula:



	<b>5-ATZ</b>
Formula	CH <sub>3</sub> N <sub>5</sub>
Molecular mass [g mol <sup>-1</sup> ]	85.07
Appearance at RT	White powder <sup>[4]</sup> , colorless rectangular prisms <sup>[5]</sup> , crystallizes as shiny leaves or large prisms <sup>[13]</sup> , crystalline solid <sup>[15]</sup> , colorless solid <sup>[17]</sup>
<i>N</i> [%]	82.33
$\Omega(\text{CO}_2)$ [%]	-65.8
<i>T</i> <sub>m.p.</sub> [°C]	480 K <sup>[4]</sup> , 205 (onset, FT-IR) <sup>[8]</sup> , 476 K <sup>[10]</sup> , 478 K <sup>[10,11]</sup> , 210 (endo, DSC @ 10 °C/min) <sup>[12]</sup> , 199 <sup>[13]</sup> , ~205 (anhydrous ATZ) <sup>[14]</sup> , 205–207 <sup>[15]</sup> , 478 K (@ 10 K/min) <sup>[16]</sup> , 473 K (microcalorimeter) <sup>[16]</sup> , 202 (with dec., onset, DSC @ 5 °C/min, covered Al container) <sup>[17]</sup>
<i>T</i> <sub>phase transition</sub> [°C]	Orthorhombic phase stable up to 11.6 GPa <sup>[4]</sup> , 5ATZ·H <sub>2</sub> O has one crystal phase (monoclinic, P2 <sub>1</sub> /c) <sup>[14]</sup> , three anhydrous crystal phases (I, II, III) up to its mpt. <sup>[14]</sup> , phase transitions accompanied by sublimation @ 175 °C: phase I → phase II required 13 h @ 175 °C, phase II → phase III required 87 h @ 175 °C <sup>[14]</sup>

$T_{\text{dehydration}}$ [°C]	~50 (monohydrate crystal) <sup>[14]</sup> , 480 K (@ 10 K/min) <sup>[16]</sup> Dehydration $T$ and enthalpies at various heating rates, $T_o$ = onset temperature, $T_p$ = peak temperature and $T_e$ = end temperature <sup>[14]</sup> :																												
	<table border="1"> <thead> <tr> <th rowspan="2">Heating rate (K/min)</th> <th colspan="3"><math>T</math> (°C)</th> <th rowspan="2"><math>\Delta H</math> (kcal/mol)</th> </tr> <tr> <th><math>T_o</math></th> <th><math>T_p</math></th> <th><math>T_e</math></th> </tr> </thead> <tbody> <tr> <td>5</td><td><math>51.2 \pm 1.8</math></td><td><math>68.2 \pm 1.4</math></td><td><math>73.4 \pm 0.8</math></td><td><math>12.7 \pm 0.2</math></td></tr> <tr> <td>10</td><td><math>52.4 \pm 1.0</math></td><td><math>73.7 \pm 1.4</math></td><td><math>81.8 \pm 1.6</math></td><td><math>12.1 \pm 0.2</math></td></tr> <tr> <td>15</td><td><math>53.4 \pm 1.8</math></td><td><math>76.9 \pm 1.1</math></td><td><math>86.2 \pm 0.6</math></td><td><math>12.2 \pm 0.1</math></td></tr> <tr> <td>20</td><td><math>55.5 \pm 1.0</math></td><td><math>80.0 \pm 1.1</math></td><td><math>91.9 \pm 1.2</math></td><td><math>11.7 \pm 0.8</math></td></tr> </tbody> </table>	Heating rate (K/min)	$T$ (°C)			$\Delta H$ (kcal/mol)	$T_o$	$T_p$	$T_e$	5	$51.2 \pm 1.8$	$68.2 \pm 1.4$	$73.4 \pm 0.8$	$12.7 \pm 0.2$	10	$52.4 \pm 1.0$	$73.7 \pm 1.4$	$81.8 \pm 1.6$	$12.1 \pm 0.2$	15	$53.4 \pm 1.8$	$76.9 \pm 1.1$	$86.2 \pm 0.6$	$12.2 \pm 0.1$	20	$55.5 \pm 1.0$	$80.0 \pm 1.1$	$91.9 \pm 1.2$	$11.7 \pm 0.8$
Heating rate (K/min)	$T$ (°C)			$\Delta H$ (kcal/mol)																									
	$T_o$	$T_p$	$T_e$																										
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10	$52.4 \pm 1.0$	$73.7 \pm 1.4$	$81.8 \pm 1.6$	$12.1 \pm 0.2$																									
15	$53.4 \pm 1.8$	$76.9 \pm 1.1$	$86.2 \pm 0.6$	$12.2 \pm 0.1$																									
20	$55.5 \pm 1.0$	$80.0 \pm 1.1$	$91.9 \pm 1.2$	$11.7 \pm 0.8$																									
$T_{\text{dec.}}$ [°C]	$\geq 206^{[2]}$ , 215 (bubbles and dec., FT-IR) <sup>[8]</sup> , dec. begins just after melting @ 480 K (TG @ 10 K/min) <sup>[10]</sup> , 495 K (TG, weak exotherm, open holder) <sup>[10]</sup> , 490–600 K (DTA, strong exotherm, hermetic holder under self-generated atmosphere) <sup>[10]</sup> , 573 K (reaction time = 0.3 ms, MS @ 560,000 K/s) <sup>[16]</sup> , 202 (with dec., onset, DSC @ 5 °C/min, covered Al container) <sup>[17]</sup>																												
$\rho$ [g cm <sup>-3</sup> ]																													
Heat of formation	209.2 kJ/mol (enthalpy of form.) <sup>[2]</sup> , $323.8 \pm 2.6$ kJ/mol ( $\Delta H_f^\circ(g)$ ) <sup>[7]</sup> , $207.8 \pm 2.3$ kJ/mol ( $\Delta H_f^\circ(s)$ ) <sup>[7]</sup> , 49.7 kcal/mol ( $\Delta_fH^\circ_{\text{solid}}$ ) <sup>[15]</sup> , 77.5 kcal/mol ( $\Delta_fH^\circ_{\text{gas}}$ , exptl.) <sup>[15]</sup> , 81.5 kcal/mol ( $\Delta_fH^\circ_{\text{gas}}$ , calcd., G3 method) <sup>[15]</sup> , 81.8 kcal/mol ( $\Delta_fH^\circ_{\text{gas}}$ , calcd., B3LYP method) <sup>[15]</sup>																												
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.																										
$-\Delta_{\text{ex}}U^\circ$ [kJ kg <sup>-1</sup> ]																													
$T_{\text{ex}}$ [K]																													
$p_{\text{C-J}}$ [kbar]																													
VoD [m s <sup>-1</sup> ]																													
$V_0$ [L kg <sup>-1</sup> ]																													
Thermal stability	50% mass loss @ 480–540 K and 100% mass loss @ 1,000 K <sup>[10]</sup> , 50% mass loss @ 480–540 K <sup>[11]</sup>																												
Burn rate [mm/s]	Values from Russian FLAME database <sup>[1]</sup> : 0.3 mm/s @ 10 atm <sup>[1]</sup> , 1.0 mm/s @ 25 atm <sup>[1]</sup> , 5.0 mm/s @ 100 atm <sup>[1]</sup> , 10.0 mm/s @ 400 atm <sup>[1]</sup> , 0.55 mm/s @ 1.2 MPa <sup>[9]</sup> , 0.95 mm/s @ 2 MPa <sup>[9]</sup> , 0.65 mm/s @ 2.1 MPa <sup>[9]</sup> , 0.9 mm/s @ 3.1 MPa <sup>[9]</sup> , 1.8 mm/s @ 4 MPa <sup>[9]</sup> , 1.9 mm/s @ 4.5 MPa <sup>[9]</sup> , 3 mm/s @ 5 MPa <sup>[9]</sup> , 4 mm/s @ 6 MPa <sup>[9]</sup> , 4.5 mm/s @ 10 MPa <sup>[9]</sup> , 7 mm/s @ 10 MPa <sup>[9]</sup> , 8 mm/s @ 16 MPa <sup>[9]</sup> , 9 mm/s @ 20 MPa <sup>[9]</sup> , 6.5 mm/s @ 20 MPa <sup>[9]</sup> , 10 mm/s @ 25 MPa <sup>[9]</sup> , 12 mm/s @ 35 MPa <sup>[9]</sup>																												

Solubility [g/mL]	Recryst. from $\text{H}_2\text{O}$ <sup>[5,10]</sup> , low solubility in organic solvents such as $\text{CH}_2\text{Cl}_2$ , $\text{Et}_2\text{O}$ <sup>[17]</sup> , only slightly soluble in cold alcohols and water <sup>[17]</sup>
Hygroscopicity	Hygroscopic, anhydrous 5-ATZ absorbs moisture from the atmosphere to form the monohydrate <sup>[4]</sup> , not hygroscopic <sup>[17]</sup>
$\Delta H_{\text{sub}}$ [kJ/mol]	112.6 (exptl.) <sup>[3]</sup> , 122.8 (calcd., QSPR) <sup>[3]</sup> , $116.0 \pm 1.2$ <sup>[7]</sup> , 116.0 <sup>[7]</sup> , $\Delta H_{\text{sub}}^{\circ} = 27.8$ kcal/mol <sup>[15]</sup>
Burning $T$ [ $^{\circ}\text{C}$ ]	1,747 K (adiabatic burning temperature @ 30 MPa) <sup>[9]</sup>
$\Delta H_{\text{dec}}$ [kJ mol <sup>-1</sup> ]	-8.5 (DSC @ 10 K/min, 10 atm $\text{N}_2$ pressure, 480–610 K) <sup>[11]</sup>
$\Delta H_{\text{dehydration}}$ [kJ mol <sup>-1</sup> ]	12.2 kcal/mol (ATZ•monohydrate) <sup>[14]</sup>

	5-ATZ <sup>[4]</sup>	5-ATZ• $\text{H}_2\text{O}$ <sup>[5]</sup>	5-ATZ• $\text{H}_2\text{O}$ <sup>[6]</sup>	5-ATZ• $\text{H}_2\text{O}$ <sup>[17]</sup>
Chemical formula	$\text{CH}_3\text{N}_5$	$\text{CH}_2\text{N}_5\text{O}$	$\text{CH}_2\text{N}_5\text{O}$	$\text{CH}_3\text{H}_5 \bullet \text{H}_2\text{O}$
Molecular weight [g mol <sup>-1</sup> ]	85.07	103.10	103.10	103.10
Crystal system	Orthorhombic	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_12_12_1$ (19)	$P2_1/c$ (14)	$P2_1/c$ (14)	$P2_1/c$ (14)
$a$ [\mathring{A}]	5.0900	6.410(20)	6.392(1)	6.389(4)
$b$ [\mathring{A}]	3.6663	7.290(20)	7.277(2)	7.198(5)
$c$ [\mathring{A}]	18.0741	9.850(20)	9.803(2)	9.198(5)
$\alpha$ [ $^{\circ}$ ]	90	90	90	90
$\beta$ [ $^{\circ}$ ]	90	90.25(17)	90.24(2)	90.198(5)
$\gamma$ [ $^{\circ}$ ]	90	90	90	90
$V$ [\mathring{A} <sup>3</sup> ]	337.29	460.275	455.978	451.6(5)
$Z$	4	4	4	4
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]		1.488	1.502	1.516
$T$ [K]	298	295	295	200
	X-ray powder diffraction	ATZ	ATZ	ATZ

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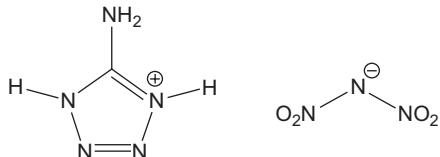
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## 5-Aminotetrazolium dinitramide

Name [German, acronym]: Aminotetrazolium dinitramide, 5-aminotetrazolium dinitramide [5-aminotetrazolium dinitramid, HAT-DN]

Main (potential) use: Possible future component of high-explosive formulations<sup>[2]</sup>, possible gas-generating agent<sup>[2]</sup>

### Structural formula:



HAT-DN			
Formula	$\text{CH}_4\text{N}_8\text{O}_4$		
Molecular mass [g mol <sup>-1</sup> ]	192.09		
Appearance at RT	Colorless rod crystals <sup>[2]</sup>		
IS [J]	2 (BAM) <sup>[2]</sup> , 2 (75–125 $\mu\text{m}$ grain size, BAM) <sup>[4]</sup>		
FS [N]	20 (BAM) <sup>[2]</sup> , 20 (75–125 $\mu\text{m}$ grain size, BAM) <sup>[4]</sup>		
ESD [J]	750 mJ (5–100 $\mu\text{m}$ crystal size, OZM apparatus) <sup>[2,4]</sup>		
N [%]	58.33		
$\Omega(\text{CO}_2)$ [%]	0		
$T_{\text{m.p.}}$ [°C]	85 (endo, onset, DSC @ 5 K/min, pressed Al container with hole in lid) <sup>[2,4]</sup>		
$T_{\text{dec.}}$ [°C]	117 (DSC @ 10 °C/min) <sup>[1]</sup> , 251 ± 7 (onset dec., T, MS @ 326,000 K/s; 0.7 ms reaction time) <sup>[1]</sup> , 117 (exo, onset, DSC @ 5 K/min, pressed Al container with hole in lid) <sup>[2,4]</sup> , 693 K (reaction time = 0.7 ms, MS @ 560,000 K/s) <sup>[3]</sup>		
$\rho$ [g cm <sup>-3</sup> ]	1.856 (X-ray, crystal) <sup>[2,4]</sup>		
Heat of formation	78.6 kcal/mol ( $\Delta_f H^\circ_{\text{(solid)}}$ , calcd., CBS-4M) <sup>[2,4]</sup> , 1,813.3 kJ/kg ( $\Delta_f U^\circ_{\text{(solid)}}$ , calcd., CBS-4M) <sup>[2]</sup> , 328 kJ/mol ( $\Delta H_f^\circ$ ) <sup>[4]</sup>		
Calcd. (EXPLO5 5.02)	Lit. values		Exptl.
$-\Delta_{\text{ex}} U^\circ$ [kJ kg <sup>-1</sup> ]	6,186 (@ 1.856 g cm <sup>-3</sup> ) <sup>[2,4]</sup>		
$T_{\text{ex}}$ [K]	4,657 (@ 1.856 g cm <sup>-3</sup> ) <sup>[2,4]</sup>		
$p_{\text{C-J}}$ [kbar]	384 (@ 1.856 g cm <sup>-3</sup> ) <sup>[2,4]</sup>		

VoD [ $\text{m s}^{-1}$ ]	9,429 (@ 1.856 g $\text{cm}^{-3}$ ) <sup>[2,4]</sup>		9,200 ± 500 (no $\rho$ given, Koenen test, high-speed camera) <sup>[2,4]</sup>
$V_0$ [L $\text{kg}^{-1}$ ]	822 (@ 1.856 g $\text{cm}^{-3}$ ) <sup>[2,4]</sup>		
Solubility [g/mL]	Soluble in MeOH, EtOH <sup>[2]</sup> , recryst. from EtOH <sup>[4]</sup>		
Koenen test	Rupture of steel tube into partly powder-like pieces (26.0 g sample, closing plate orifice = 10 mm, explosion within 1 ms) <sup>[2]</sup> , ≥10 mm (hole width of steel sleeve) <sup>[4]</sup>		

	HAT-DN <sup>[2]</sup>
Chemical formula	$\text{CH}_4\text{N}_8\text{O}_4$
Molecular weight [g mol <sup>-1</sup> ]	192.12
Crystal system	Monoclinic
Space group	$Pc$ (no. 7)
$a$ [\mathring{A}]	4.6283(3)
$b$ [\mathring{A}]	9.4580(6)
$c$ [\mathring{A}]	9.0071(5)
$\alpha$ [°]	90
$\beta$ [°]	119.343(4)
$\gamma$ [°]	90
$V$ [\mathring{A} <sup>3</sup> ]	343.70(4)
$Z$	2
$\rho_{\text{calc}}$ [g $\text{cm}^{-3}$ ]	1.856
$T$ [K]	200
	Crystals obtained from evaporation of an EtOH soln.

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[3] N. W. Piekel, R. E. Cavicchi, M. R. Zachariah, *Initiation and Decomposition of Green Energetic Materials*, Technical Report, U.S. Army Research Office, NC, USA.

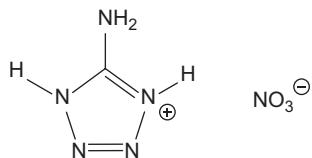
[4] J. Stierstorfer, *Advanced Energetic Materials Based on 5-Aminotetrazole – Synthesis, Characterization and Scale-Up*, PhD Thesis, LMU München, Munich, **2009**.

## 5-Aminotetrazolium nitrate

Name [German, acronym]: Aminotetrazolium nitrate, 5-amino-1*H*-tetrazole nitrate, 5-amino-1*H*-tetrazole hydronitrate [5-aminotetrazolium nitrat, 5-ATN, 5-ATEZN]

Main (potential) use: Azide-free gas-generating pyrotechnic composition<sup>[1]</sup>, potential applications in propellants and gun powders<sup>[2]</sup>, inflating air bags and actuating seatbelt pretensioners<sup>[3]</sup>

Structural formula:



	<b>5-ATN</b>														
Formula	CH <sub>4</sub> N <sub>6</sub> O <sub>3</sub>														
Molecular mass [g mol <sup>-1</sup> ]	148.08														
Appearance at RT	Colorless crystals <sup>[3]</sup> , feathery white crystals <sup>[4]</sup>														
IS [J]	<p>20–40 mg sample, all BAM method, all unexploded samples subsequently detonated @ 10 Nm<sup>[4]</sup>:</p> <table border="1"> <thead> <tr> <th>Value (Nm)</th><th>Comment</th></tr> </thead> <tbody> <tr> <td>8</td><td>&lt;0.4 mm, 6 tests, 0 explosions</td></tr> <tr> <td>9</td><td>&lt;0.4 mm, 6 tests, 2 explosions</td></tr> <tr> <td>5</td><td>0.5–1.0 mm, 6 tests, 0 explosions</td></tr> <tr> <td>6</td><td>0.5–1.0 mm, 6 tests, 1 explosion</td></tr> <tr> <td>6</td><td>&gt;1.0 mm, 6 tests, 0 explosions</td></tr> <tr> <td>7</td><td>&gt;1.0 mm, 6 tests, 1 explosion</td></tr> </tbody> </table>	Value (Nm)	Comment	8	<0.4 mm, 6 tests, 0 explosions	9	<0.4 mm, 6 tests, 2 explosions	5	0.5–1.0 mm, 6 tests, 0 explosions	6	0.5–1.0 mm, 6 tests, 1 explosion	6	>1.0 mm, 6 tests, 0 explosions	7	>1.0 mm, 6 tests, 1 explosion
Value (Nm)	Comment														
8	<0.4 mm, 6 tests, 0 explosions														
9	<0.4 mm, 6 tests, 2 explosions														
5	0.5–1.0 mm, 6 tests, 0 explosions														
6	0.5–1.0 mm, 6 tests, 1 explosion														
6	>1.0 mm, 6 tests, 0 explosions														
7	>1.0 mm, 6 tests, 1 explosion														
FS [N]	<p>&gt;324<sup>[2]</sup></p> <p>All using BAM method<sup>[4]</sup>:</p> <table border="1"> <thead> <tr> <th>Value (N)</th><th>Comments</th></tr> </thead> <tbody> <tr> <td>&gt;360</td><td>&lt;0.4 mm, 8 tests, 0 explosions @ 360 N</td></tr> <tr> <td>&gt;324</td><td>0.5–1.0 mm, 4 tests, 1 explosion @ 360 N</td></tr> <tr> <td></td><td>0.5–1.0 mm, 4 tests, 0 explosions @ 324 N</td></tr> <tr> <td>&gt;324</td><td>&gt;1.0 mm, 4 tests, 2 explosions @ 360 N</td></tr> <tr> <td></td><td>&gt;1.0 mm, 4 tests, 0 explosions @ 324 N</td></tr> </tbody> </table>	Value (N)	Comments	>360	<0.4 mm, 8 tests, 0 explosions @ 360 N	>324	0.5–1.0 mm, 4 tests, 1 explosion @ 360 N		0.5–1.0 mm, 4 tests, 0 explosions @ 324 N	>324	>1.0 mm, 4 tests, 2 explosions @ 360 N		>1.0 mm, 4 tests, 0 explosions @ 324 N		
Value (N)	Comments														
>360	<0.4 mm, 8 tests, 0 explosions @ 360 N														
>324	0.5–1.0 mm, 4 tests, 1 explosion @ 360 N														
	0.5–1.0 mm, 4 tests, 0 explosions @ 324 N														
>324	>1.0 mm, 4 tests, 2 explosions @ 360 N														
	>1.0 mm, 4 tests, 0 explosions @ 324 N														

$N$ [%]	57.3														
$\Omega(\text{CO}_2)$ [%]	-18														
$T_{\text{m.p.}}$ [°C]	No melting observed <sup>[3]</sup> , 173 (dec., Buechi melting point apparatus) <sup>[4]</sup>														
$T_{\text{dec.}}$ [°C]	183.88 (DSC @ 5 °C/min) <sup>[1]</sup> , 190.32 (DSC @ 10 °C/min) <sup>[1]</sup> , 194.04 (DSC @ 15 °C/min) <sup>[1]</sup> , 199.19 (DSC @ 20 °C/min) <sup>[1]</sup> , 177.6 (exo., peak max., DSC @ 10 °C/min, stainless steel crucible) <sup>[2]</sup> , 193 (onset, exo), 198 (exo, peak max.) (DSC @ 10 °C/min) <sup>[3]</sup> , 191 (max. rate of mass loss of 7.1%, mass loss of 18.0% @ 171–202 °C; second dec. occurs @ 224–238 °C with peak max @ 234 °C with 26.8% mass loss @ 210–270 °C, DTG-TG @ 10 °C/min) <sup>[3]</sup>  Peak $T$ of first exotherm at different heating rates, DSC (sealed Al pans) <sup>[3]</sup> :														
	<table border="1"> <thead> <tr> <th>Heating rate (°C/min)</th> <th>Peak <math>T</math> (°C)</th> </tr> </thead> <tbody> <tr> <td>2</td> <td>191.1 ± 0.2</td> </tr> <tr> <td>5</td> <td>193.6 ± 0.3</td> </tr> <tr> <td>10</td> <td>198.5 ± 0.3</td> </tr> <tr> <td>15</td> <td>200.1 ± 0.5</td> </tr> <tr> <td>20</td> <td>203.0 ± 0.4</td> </tr> <tr> <td>25</td> <td>205.2 ± 0.3</td> </tr> </tbody> </table>	Heating rate (°C/min)	Peak $T$ (°C)	2	191.1 ± 0.2	5	193.6 ± 0.3	10	198.5 ± 0.3	15	200.1 ± 0.5	20	203.0 ± 0.4	25	205.2 ± 0.3
Heating rate (°C/min)	Peak $T$ (°C)														
2	191.1 ± 0.2														
5	193.6 ± 0.3														
10	198.5 ± 0.3														
15	200.1 ± 0.5														
20	203.0 ± 0.4														
25	205.2 ± 0.3														
	169 (exo, DSC @ 2 K/min) <sup>[4]</sup> , 173 (melting with dec., Buechi melting point apparatus) <sup>[4]</sup>														
$\rho$ [g cm <sup>-3</sup> ]	1.847 <sup>[2]</sup>														
Heat of formation	87 kJ mol <sup>-1</sup> (molar heat of form.) <sup>[2,4]</sup> , 586 kJ/kg ( $\Delta_f H^\circ$ , calcd.) <sup>[4]</sup>														
Heat of combustion	-1,051 (calcd.) <sup>[4]</sup> , -6,020 ± 200 kJ/kg (exptl., bomb calorimetry) <sup>[4]</sup>														
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.												
$-\Delta_{\text{ex}} U^\circ$ [kJ kg <sup>-1</sup> ]		4,603 (calcd., K-W) <sup>[4]</sup>													
$T_{\text{ex}}$ [K]															
$p_{\text{C-J}}$ [kbar]		35.7 GPa (calcd., K-J) <sup>[4]</sup>													
$\text{VoD}$ [m s <sup>-1</sup> ]		8,898 (@ 1.847 g cm <sup>-3</sup> , calcd. K-J) <sup>[4]</sup>													
$V_0$ [L kg <sup>-1</sup> ]															

Solubility [g/mL]	Soluble in DMSO <sup>[4]</sup> recryst. from H <sub>2</sub> O <sup>[3]</sup>							
Hygroscopicity	Low hygroscopicity <sup>[1]</sup>							
Photosensitivity	Dec. in bright light, should be stored in darkness <sup>[2]</sup>							
Compatibility	DSC @ 10 °C/min, stainless steel crucible, $T_{dE}$ = exo. peak max of 5-ATN, $T_{dM}$ = peak max. of ATN admixture, $\Delta T_p = T_{dE} - T_{dM}$ , F <sub>2604-2</sub> = type of fluorinated rubber, DOS = dioctyl sebacate <sup>[2]</sup> :							
BMs	$T_{dE}$ (°C)	$T_{dM}$ (°C)	$\Delta T_p$ (°C)	Compatibility				
5-ATN/TNT	177.6	179.4	-1.8	Compatible				
5-ATN/RDX	177.6	177.4	0.2	Compatible				
5-ATN/HMX	177.6	182.2	-4.6	Compatible				
5-ATN/AP	177.6	171.7	5.9	Partially compatible				
5-ATN/CL-20	177.6	176.9	0.7	Compatible				
5-ATN/Al	177.6	174.8	2.8	Compatible				
5-ATN/F <sub>2604-2</sub>	177.6	176.0	1.6	Compatible				
5-ATN/DOS	177.6	174.2	3.4	Compatible				
VST @ 100 °C for 40 h in an initial vacuum, F <sub>2604-2</sub> = type of fluorinated rubber, DOS = dioctyl sebacate <sup>[2]</sup> :								
BMs	Evolved gas (mL/g)		Compatibility judgment					
5-ATN/TNT	-1.58		Compatible					
5-ATN/RDX	-6.49		Compatible					
5-ATN/HMX	-6.11		Compatible					
5-ATN/AP	0.43		Compatible					
5-ATN/CL-20	-5.05		Compatible					
5-ATN/Al	-2.40		Compatible					
5-ATN/F <sub>2604-2</sub>	-2.30		Compatible					
5-ATN/DOS	-1.62		Compatible					
X-ray powder diffraction <sup>[2]</sup> : 5-ATN/AP compatibility unclear but probably compatible <sup>[2]</sup> 5-ATN/TNT = compatible <sup>[2]</sup> , 5-ATN/RDX = compatible <sup>[2]</sup> , 5-ATN/HMX = compatible <sup>[2]</sup> , 5-ATN/CL-20 = compatible <sup>[2]</sup> IR spectroscopy <sup>[2]</sup> : 5-ATN/TNT = compatible <sup>[2]</sup> , 5-ATN/RDX = compatible <sup>[2]</sup> , 5-ATN/CL-20 = compatible <sup>[2]</sup> , 5-ATN/Al = compatible <sup>[2]</sup> , 5-ATN/F <sub>2604-2</sub> = compatible <sup>[2]</sup> , 5-ATN-DOS = compatible <sup>[2]</sup>								
$\Delta H_{dec}$ [J/g]	246 (DSC @ 10 °C/min) <sup>[3]</sup>							
Koenen test	Critical diameter >10 mm (25 g sample compacted with 80 N) <sup>[4]</sup>							

	<b>5-ATZN<sup>[3]</sup></b>	<b>5-ATZN<sup>[4]</sup></b>
Chemical formula	CH <sub>4</sub> N <sub>6</sub> O <sub>3</sub>	CH <sub>4</sub> N <sub>6</sub> O <sub>3</sub>
Molecular weight [g mol <sup>-1</sup> ]	148.1	148.08
Crystal system	Monoclinic	Monoclinic
Space group	<i>P</i> 2 <sub>1</sub> / <i>c</i>	<i>P</i> 2 <sub>1</sub> / <i>c</i>
<i>a</i> [Å]	10.606(2)	10.5493(8)
<i>b</i> [Å]	3.5065(4)	3.4556(4)
<i>c</i> [Å]	14.641(2)	14.606(1)
$\alpha$ [°]	90	90
$\beta$ [°]	90.63(1)	90.548(9)
$\gamma$ [°]	90	90
<i>V</i> [Å <sup>3</sup> ]	544.4(1)	532.44(8)
<i>Z</i>	4	4
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.807	1.847
<i>T</i> [K]	296	200
	Crystals from slow evaporation of aqueous soln. @ RT	

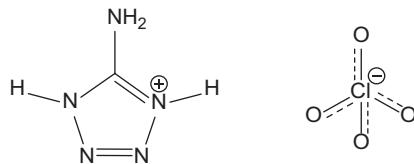
- [1] T. Xu, Z. Du, M. Wang, *Adv. Mater. Res.*, **2014**, *1004–1005*, 719–725.
- [2] W. Guo, Z. Han, Q. Lin, B. Wang, *Centr. Eur. J. Energet. Mater.*, **2018**, *15*, 100–114.
- [3] G. Ma, T. Zhang, J. Zhang, K. Yu, *Thermochim. Acta*, **2004**, *423*, 137–141.
- [4] M. von Denffer, T. M. Klapötke, G. Kramer, G. Spieß, J. M. Welch, *Propellants, Explosives, Pyrotechnics*, **2005**, *30*, 191–195.

## 5-Amino-1*H*-tetrazolium perchlorate

Name [German, acronym]: 5-Aminotetrazolium perchlorate, aminotetrazolium perchlorate, [5-aminotetrazolium perchlorat]

Main (potential) use: oxidizer

Structural formula:



	<b>Aminotetrazolium perchlorate</b>		
Formula	$\text{CH}_4\text{N}_4\text{O}_4\text{Cl}$		
Molecular mass [g mol <sup>-1</sup> ]	185.53		
Appearance at RT	Colorless platelets (recryst. from $\text{H}_2\text{O}$ ) <sup>[1]</sup>		
IS [J]	1.5 (BAM) <sup>[1]</sup>		
FS [N]	8 (BAM) <sup>[1]</sup>		
ESD [J]			
N [%]	37.75		
$\Omega(\text{CO}_2)$ [%]			
$T_{\text{m.p.}}$ [ $^\circ\text{C}$ ]	176 (DSC, onset @ 2 $^\circ\text{C}/\text{min}$ ) <sup>[1]</sup>		
$T_{\text{dec.}}$ [ $^\circ\text{C}$ ]	~180 (DSC, onset @ 2 $^\circ\text{C}/\text{min}$ ) <sup>[1]</sup>		
$\rho$ [g cm <sup>-3</sup> ]			
Heat of formation			
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^\circ$ [kJ kg <sup>-1</sup> ]			
$T_{\text{ex}}$ [K]			
$p_{\text{CJ}}$ [kbar]			
$\text{VoD}$ [m s <sup>-1</sup> ]			
$V_0$ [L kg <sup>-1</sup> ]			
Critical diameter [cm]			
Trauzl test [cm <sup>3</sup> , % TNT]			

Sand test [g]	
Ballistic mortar test	
LSGT [cm]	
SSGT [cm]	
5 s explosion $T$ [°C]	
100 °C heat test [% mass loss]	
Thermal stability	
Vacuum stability test [cm <sup>3</sup> /h]	
Vapor pressure [Pa]	
Burn rate [mm/s]	
Solubility [g/mL]	Soluble in DMSO, MeOH <sup>[1]</sup> , recryst. from H <sub>2</sub> O <sup>[1]</sup>
Hygroscopicity	
Photosensitivity	
Compatibility	
$K_{ow}$ (log)	

	<b>5-Aminotetrazolium perchlorate<sup>[1]</sup></b>
Chemical formula	CH <sub>4</sub> N <sub>5</sub> O <sub>4</sub> Cl
Molecular weight [g mol <sup>-1</sup> ]	185.53
Crystal system	
Space group	
$a$ [Å]	
$b$ [Å]	
$c$ [Å]	
$\alpha$ [°]	
$\beta$ [°]	
$\gamma$ [°]	
$V$ [Å <sup>3</sup> ]	
$Z$	
$\rho_{calc}$ [g cm <sup>-3</sup> ]	
$T$ [K]	

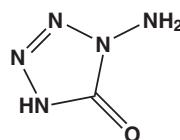
[1] J. Stierstorfer, *Advanced Energetic Materials Based on 5-Aminotetrazole – Synthesis, Characterization and Scale-Up*, PhD Thesis, LMU München, Munich, 2009.

## 1-Aminotetrazol-5-one

Name [German, acronym]: 1-Aminotetrazol-5-one [1-Aminotetrazol-5-on ATO]

Main (potential) use: Secondary (high) explosive

Structural formula:



	ATO
Formula	$\text{CH}_3\text{N}_5\text{O}$
Molecular mass [g mol <sup>-1</sup> ]	101.08
Appearance at RT	
IS [J]	>40 <sup>[1]</sup>
N [%]	69.29
$\Omega(\text{CO})$ [%]	-23.76
$T_{\text{m.p.}}$ [°C]	221.0 (endo, peak max., DSC-TG @ 10 °C/min) <sup>[1]</sup>
$T_{\text{dec.}}$ [°C]	227.1 (DSC-TG @ 10 °C/min) <sup>[1]</sup>
$\rho$ [g cm <sup>-3</sup> ]	1.796 (crystal, @ 298 K) <sup>[1]</sup>
Heat of formation	342.98 kJ/mol ( $\Delta_f H^\circ$ , calcd.) <sup>[1]</sup> , 3,395.8 kJ kg <sup>-1</sup> ( $\Delta_f H^\circ$ , calcd.) <sup>[1]</sup>
$-\Delta_{\text{ex}} U^\circ$ [kJ kg <sup>-1</sup> ]	
$T_{\text{ex}}$ [K]	
$p_{\text{C-J}}$ [GPa]	35.0 <sup>[1]</sup>
VoD [m s <sup>-1</sup> ]	8,880 <sup>[1]</sup>
$V_0$ [L kg <sup>-1</sup> ]	
Solubility [g/mL]	Insoluble in EtOH <sup>[1]</sup> , soluble in benzaldehyde <sup>[1]</sup>

	<b>ATO<sup>[1]</sup></b>
Chemical formula	CH <sub>3</sub> N <sub>5</sub> O
Molecular weight [g mol <sup>-1</sup> ]	101.08
Crystal system	Orthorhombic
Space group	<i>Pbca</i> (61)
<i>a</i> [Å]	9.8873(7)
<i>b</i> [Å]	5.5314(3)
<i>c</i> [Å]	13.6734(9)
$\alpha$ [°]	90
$\beta$ [°]	90
$\gamma$ [°]	90
<i>V</i> [Å <sup>3</sup> ]	747.81(8)
<i>Z</i>	8
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.796
<i>T</i> [K]	298

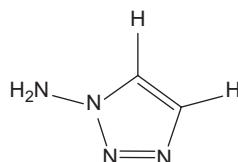
- [1] X. Yin, J.-T. Wu, X. Jin, C.-X. Xu, P. He, T. Li, K. Wang, J. Qin, J.-G. Zhang, *RSC Adv.*, **2015**, *5*, 60,005–60,014.

## 1-Amino-1,2,3-triazole

Name [German, acronym]: Aminotriazole, [1-Amino-1,2,3-triazol, ATZ]

Main (potential) use: gas generant

Structural formula:



	1-Amino-1,2,3-triazole		
Formula	$\text{C}_2\text{H}_4\text{N}_4$		
Molecular mass [g mol <sup>-1</sup> ]	84.08		
Appearance at RT			
IS [J]			
FS [N]			
ESD [J]			
N [%]	66.63		
$\Omega(\text{CO}_2)$ [%]	-114.2		
$T_{\text{m.p.}}$ [ $^{\circ}\text{C}$ ]	49–50 <sup>[1,2,3]</sup>		
$T_{\text{b.p.}}$ [ $^{\circ}\text{C}$ ]	124–125 (@6 mm HG) <sup>[3]</sup>		
$T_{\text{phase transition}}$ [ $^{\circ}\text{C}$ ]			
$T_{\text{dec.}}$ [ $^{\circ}\text{C}$ ]			
$\rho$ [g cm <sup>-3</sup> ]	1.484 (crystal @100 K) <sup>[1]</sup>		
Heat of formation	285.6		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^\circ$ [kJ kg <sup>-1</sup> ]	3772		
$T_{\text{ex}}$ [K]	2404		
$p_{\text{C-J}}$ [kbar]	19.5		
VoD [m s <sup>-1</sup> ]	7767		
$V_0$ [L kg <sup>-1</sup> ]	813		

Solubility [g/mL]	soluble in H <sub>2</sub> O, EtOH, OMSO <sup>[3]</sup>
Hygroscopicity	

	1-Amino-1,2,3-triazole <sup>[1]</sup>
Chemical formula	C <sub>2</sub> H <sub>4</sub> N <sub>4</sub>
Molecular weight [g mol <sup>-1</sup> ]	84.09
Crystal system	Orthorhombic
Space group	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub> (no. 19)
a [Å]	5.566(2)
b [Å]	6.865(2)
c [Å]	9.847(4)
α [°]	90
β [°]	90
γ [°]	90
V [Å <sup>3</sup> ]	376.3(2)
Z	4
ρ <sub>calc</sub> [g cm <sup>-3</sup> ]	1.484
T [K]	100

[1] G. Kaplan, G. Drake, K. Tollison, L. Hall, T. Hawkins, *J. Heterocyclic Chem.*, **2005**, 42, 19–27.

[2] Q.-H. Lin, Y.-C. Li, Y.-Y. Li, Z. Wang, W. Liu, C. Qi, S.-P. Pang, *J. Mater. Chem.*, **2012**, 22, 666–674.

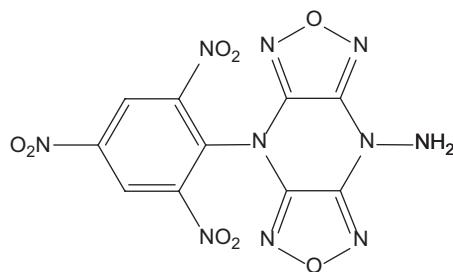
[3] K. Shigeno, T. Ono, M. Tanaka, S. Yamada, T. Asao, Process for Preparing 1-Amino-1,2,3-Triazole, US Patent 5,728,841, 17th March 1998.

## 4-Amino-8-(2,4,6-trinitrophenyl)difurazano[3,4-*b*:3',4'-*e*]pyrazine

Name [German, acronym]: 4-Amino-8-(2,4,6-trinitrophenyl)difurazano[3,4-*b*:3',4'-*e*]pyrazine [4-amino-8-(2,4,6-trinitrophenyl)difurazano[3,4-*b*:3',4'-*e*]pyrazin]

Main (potential) use: Potential new heat-resistant explosive<sup>[1]</sup>

Structural formula:



	<b>4-Amino-8-(2,4,6-trinitrophenyl)difurazano[3,4-<i>b</i>:3',4'-<i>e</i>]pyrazine</b>		
Formula	C <sub>10</sub> H <sub>4</sub> N <sub>10</sub> O <sub>8</sub>		
Molecular mass [g mol <sup>-1</sup> ]	392.20		
Appearance at RT	Brown powder <sup>[1]</sup>		
IS [J]	20 (ZBL-B instrument) <sup>[1]</sup>		
FS [N]	>360 (FSKM 10 instrument) <sup>[1]</sup>		
ESD [J]	3 (ESD 2008A electric spark tester) <sup>[1]</sup>		
N [%]	35.71		
Ω(CO <sub>2</sub> ) [%]	-57.1		
T <sub>dec.</sub> [°C]	283 (DSC @ 10 °C/min) <sup>[1]</sup>		
ρ [g cm <sup>-3</sup> ]	1.72 (gas pycnometer @ 25 °C) <sup>[1]</sup>		
Heat of formation	782.6 kJ/mol (ΔH <sub>f</sub> ) <sup>[1]</sup>		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
-Δ <sub>ex</sub> U° [kJ kg <sup>-1</sup> ]			
T <sub>ex</sub> [K]			

$p_{C_J}$ [kbar]		25.7 GPa (@ 1.72 g cm <sup>-3</sup> , $\Delta H_f = 782.6$ kJ/ mol, calcd., K-J) <sup>[1]</sup>	
VoD [m s <sup>-1</sup> ]		7,641 (@ 1.72 g cm <sup>-3</sup> , $\Delta H_f = 782.6$ kJ/ mol, calcd., K-J) <sup>[1]</sup>	
$V_0$ [L kg <sup>-1</sup> ]			

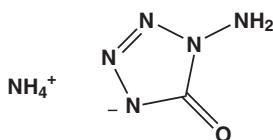
[1] N. Liu, Y.-J. Shu, H. Li, L.-J. Zhai, Y.-N. Li, B.-Z. Wang, *RSC Adv.*, **2015**, *5*, 43,780–43,785.

## Ammonium 1-aminotetrazol-5-oneate

Name [German, acronym]: Ammonium 1-aminotetrazol-5-oneate [ATO·NH<sub>3</sub>]

Main (potential) use: Secondary (high) explosive

Structural formula:



	<b>ATO · NH<sub>3</sub></b>	
Formula	$\text{CH}_6\text{N}_6\text{O}$	
Molecular mass [g mol <sup>-1</sup> ]	118.12	
Appearance at RT		
IS [J]	>40 <sup>[1]</sup>	
N [%]	75.7	
$\Omega(\text{CO}_2)$ [%]	-54.18	
$\rho$ [g cm <sup>-3</sup> ]	1.647 (crystal, @ 298 K) <sup>[1]</sup>	
Heat of formation	225.01 kJ/mol ( $\Delta_f H^\circ$ , calcd.) <sup>[1]</sup> , 1,906.9 kJ kg <sup>-1</sup> ( $\Delta_f H^\circ$ , calcd.) <sup>[1]</sup>	
	Calcd. (K-J)	Exptl.
$-\Delta_{\text{ex}} U^\circ$ [kJ kg <sup>-1</sup> ]		
$T_{\text{ex}}$ [K]		
$p_{\text{C-J}}$ [GPa]	28.7 <sup>[1]</sup>	
VoD [m s <sup>-1</sup> ]	8,260 <sup>[1]</sup>	
$V_0$ [L kg <sup>-1</sup> ]		
Thermal stability	Only stable in aqueous soln., attempts to remove water result in dec. <sup>[1]</sup> , solid crystals dec. within 2 days @ RT <sup>[1]</sup>	

	<b>ATO•NH<sub>3</sub><sup>[1]</sup></b>
Chemical formula	CH <sub>6</sub> N <sub>6</sub> O
Molecular weight [g mol <sup>-1</sup> ]	118.12
Crystal system	Monoclinic
Space group	P2 <sub>1</sub> /c (14)
<i>a</i> [Å]	10.6535(7)
<i>b</i> [Å]	6.5711(5)
<i>c</i> [Å]	6.9431(6)
$\alpha$ [°]	90
$\beta$ [°]	101.531(2)
$\gamma$ [°]	90
<i>V</i> [Å <sup>3</sup> ]	476.24(6)
<i>Z</i>	4
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.647
<i>T</i> [K]	298

[1] X. Yin, J.-T. Wu, X. Jin, C.-X. Xu, P. He, T. Li, K. Wang, J. Qin, J.-G. Zhang, *RSC Adv.*, **2015**, *5*, 60,005–60,014.

## Ammonium Azide

Name [German, acronym]: Ammonium azide [ammoniumazid, AA]

Main (potential) use: Precursor for synthesis of polymeric nitrogen<sup>[1]</sup>

**Structural formula:**



Ammonium azide																													
Formula	NH <sub>4</sub> N <sub>3</sub>																												
Molecular mass [g mol <sup>-1</sup> ]	60.06																												
Appearance at RT	Soft white crystals <sup>[9]</sup> , white crystalline (rhombic) substance <sup>[10]</sup>																												
IS [J]	<p>Nonimpact sensitive<sup>[9]</sup>, stable to steel on steel impact ≤ 12.2 kg m<sup>[9]</sup>, insensitive to 12.2 kg m impact @ 160 °C<sup>[9]</sup></p> <p>% explosions, instrument no. 4, K-44-2, drop hammer, 10 kg load, 25 cm drop height, two different locations for charge<sup>[12]</sup>:</p> <table border="1"> <thead> <tr> <th colspan="6">Weight (mg)</th> <th></th> </tr> <tr> <th colspan="3">Centrally located</th> <th colspan="3">Uniformly located</th> <th></th> </tr> <tr> <th>2</th> <th>10</th> <th>50</th> <th>2</th> <th>10</th> <th>50</th> <th>mg</th> </tr> </thead> <tbody> <tr> <td>8</td> <td>64</td> <td>0</td> <td>0</td> <td>4</td> <td>4</td> <td>%</td> </tr> </tbody> </table>	Weight (mg)							Centrally located			Uniformly located				2	10	50	2	10	50	mg	8	64	0	0	4	4	%
Weight (mg)																													
Centrally located			Uniformly located																										
2	10	50	2	10	50	mg																							
8	64	0	0	4	4	%																							
N [%]	93.29																												
Ω(CO <sub>2</sub> ) [%]	-53.3																												
T <sub>m.p.</sub> [°C]	160 (expl.), starts to sublime at 133–134, 230–240 <sup>[9]</sup> , 160 <sup>[10]</sup>																												
T <sub>dec.</sub> [°C]	Slow dec. at 250–450 °C @ 70 mm Hg <sup>[7]</sup> , slow dec. @ 25–310 °C @ 150 mm Hg <sup>[7]</sup> , sublimes then explodes on heating <sup>[10]</sup>																												
ρ [g cm <sup>-3</sup> ]	1.346 (@ 298 K) <sup>[2,7,9]</sup> , 1.3459 (crystal) <sup>[10]</sup>																												
Heat of formation	120.4 kJ/mol (enthalpy of form., calcd. emp.) <sup>[3]</sup> , 115.6 kJ/mol (enthalpy of form., exptl.) <sup>[3]</sup> , 112.8 kJ/mol <sup>[1]</sup> , 2,004.7 kJ kg <sup>-1</sup> (enthalpy of form., exptl.) <sup>[3]</sup> , 1,891.2 kJ kg <sup>-1</sup> <sup>[4]</sup> , 27 kJ/mol <sup>[9]</sup> , 27.6 kcal/mol <sup>[10]</sup> , 26.79 kcal/mol <sup>[10]</sup> , 26.4 kcal/mol <sup>[10]</sup> , -19 kcal/mol (Q <sub>c</sub> ) <sup>[7]</sup> , +27.6 kcal/mol (Δ <sub>f</sub> H <sup>o</sup> , exptl.) <sup>[8]</sup> , 28.90 kcal/mol (Δ <sub>f</sub> H <sup>o</sup> , calcd.) <sup>[8]</sup> , 112.1 kJ/mol (Δ <sub>f</sub> H <sup>o</sup> , exptl.) <sup>[13]</sup> , 179.1 kJ/mol (Δ <sub>f</sub> H <sup>o</sup> , calcd., Born–Haber cycles) <sup>[13]</sup>																												
Heat of combustion	Q <sub>c</sub> <sup>P</sup> = ~98 kcal/mol <sup>[7]</sup>																												
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.																										

$-\Delta_{\text{ex}}U^0 \text{ [kJ kg}^{-1}\text{]}$	2,938		$Q_e = 31.2 \text{ kcal/mol}^{[7]}$																																																
$T_{\text{ex}} \text{ [K]}$	2,015		1,673.2																																																
$p_{\text{C-J}} \text{ [GPa] calcd.}$	18.87	15.16 GPa (calcd., K-J) <sup>[1]</sup>																																																	
VoD [ $\text{m s}^{-1}$ ]	8,178 (@ 1.346 g $\text{cm}^{-3}$ ; $\Delta_f H = 114 \text{ kJ mol}^{-1}$ )	6,450 (@ 1.357 g $\text{cm}^{-3}$ , calcd., K-J) <sup>[1]</sup>	Effect of the charge (steel shell) on the VoD of AA (polydisperse powder with particle size $\leq 100 \mu\text{m}$ ) <sup>[10]</sup> : 2,150 (@ 0.25 g $\text{cm}^{-3}$ ) <sup>[10]</sup> , 2,600 (@ 0.50 g $\text{cm}^{-3}$ ) <sup>[10]</sup>																																																
$V_0 \text{ [L kg}^{-1}\text{]}$	1,106																																																		
Critical diameter [cm]	Dependence of critical diameter of AA on the density of the charge (determined in cellophane, or thin-walled glass shells, streak camera; approx. values taken from graph) <sup>[10]</sup> :																																																		
	<table border="1"><thead><tr><th><math>d \text{ (mm)}</math></th><th><math>\rho \text{ (g/cm}^3\text{)}</math></th><th><math>d \text{ (mm)}</math></th><th><math>\rho \text{ (g/cm}^3\text{)}</math></th></tr></thead><tbody><tr><td>9</td><td>0.4+</td><td>17.8</td><td>0.55-</td></tr><tr><td>11.5</td><td>0.44+</td><td>17.8</td><td>0.6-</td></tr><tr><td>11.5</td><td>0.48+</td><td>13.8</td><td>9.64-</td></tr><tr><td>12.5</td><td>0.45+</td><td>17.5</td><td>0.65-</td></tr><tr><td>12.5</td><td>0.52+</td><td>16.5</td><td>0.68-</td></tr><tr><td>13.5</td><td>0.54+</td><td>13.9</td><td>0.7-</td></tr><tr><td>12.5</td><td>0.55-</td><td>17.8</td><td>0.73-</td></tr><tr><td>6.5</td><td>0.48-</td><td>9.0</td><td>0.73-</td></tr><tr><td>8.2</td><td>0.49-</td><td></td><td></td></tr><tr><td>11.0</td><td>0.55-</td><td></td><td></td></tr><tr><td>15.5</td><td>0.54+</td><td></td><td></td></tr></tbody></table>	$d \text{ (mm)}$	$\rho \text{ (g/cm}^3\text{)}$	$d \text{ (mm)}$	$\rho \text{ (g/cm}^3\text{)}$	9	0.4+	17.8	0.55-	11.5	0.44+	17.8	0.6-	11.5	0.48+	13.8	9.64-	12.5	0.45+	17.5	0.65-	12.5	0.52+	16.5	0.68-	13.5	0.54+	13.9	0.7-	12.5	0.55-	17.8	0.73-	6.5	0.48-	9.0	0.73-	8.2	0.49-			11.0	0.55-			15.5	0.54+				
$d \text{ (mm)}$	$\rho \text{ (g/cm}^3\text{)}$	$d \text{ (mm)}$	$\rho \text{ (g/cm}^3\text{)}$																																																
9	0.4+	17.8	0.55-																																																
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8.2	0.49-																																																		
11.0	0.55-																																																		
15.5	0.54+																																																		
Thermal stability	Dissociates below the mpt. and the vapors are completely dissociated @ RT <sup>[11]</sup> , explodes when heated in closed system but not in open air due to pressure buildup of $\text{HN}_3$ <sup>[11]</sup>																																																		
Vapor pressure [atm @ $^{\circ}\text{C}$ ]	3.62 mm Hg @ 40 $^{\circ}\text{C}$ <sup>[9]</sup> , 6.31 mm Hg @ 60 $^{\circ}\text{C}$ <sup>[9]</sup> , 36.7 mm Hg @ 80 $^{\circ}\text{C}$ <sup>[9]</sup> , solid volatizes quickly if left uncovered <sup>[11]</sup>																																																		
Solubility [g/mL]	20 g/100 g $\text{H}_2\text{O}$ @ 20 $^{\circ}\text{C}$ <sup>[9]</sup> , limitingly soluble in water <sup>[10]</sup> , 20.16 g/100 mL $\text{H}_2\text{O}$ @ 20 $^{\circ}\text{C}$ <sup>[11]</sup> , 3.27 g/100 mL MeOH @ 20 $^{\circ}\text{C}$ <sup>[11]</sup> , 1.06 g/100 mL in EtOH @ 20 $^{\circ}\text{C}$ <sup>[11]</sup> , easily recryst. from hot MeOH or precipitated with $\text{Et}_2\text{O}$ <sup>[11]</sup>																																																		
Hygroscopicity	Nonhygroscopic <sup>[9]</sup>																																																		
Compatibility	Incompatible with Cu or other heavy metals <sup>[9]</sup> , compatible with Al <sup>[9]</sup> , stable with glass up to 300 $^{\circ}\text{C}$ <sup>[9]</sup>																																																		

	Ammonium azide <sup>[5]</sup>	Ammonium azide <sup>[6]</sup>
Chemical formula	N <sub>4</sub> H <sub>4</sub>	N <sub>4</sub> H <sub>4</sub>
Molecular weight [g mol <sup>-1</sup> ]	60.06	60.06
Crystal system	Orthorhombic	Orthorhombic
Space group	P m n a (no. 53)	P m n a (no. 53)
a [Å]	8.948(3)	8.8978(2)
b [Å]	3.808(2)	3.8067(8)
c [Å]	8.659(3)	8.6735(17)
α [°]	90	90
β [°]	90	90
γ [°]	90	90
V [Å <sup>3</sup> ]	295.05	293.78
Z	4	4
ρ <sub>calc</sub> [g cm <sup>-3</sup> ]	1.352	
T [K]		

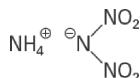
Ammonium azide crystallizes in anhydrous form from H<sub>2</sub>O.<sup>[10]</sup>

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## Ammonium dinitramide

Name [German, acronym]: Ammonium dinitramide [Ammoniumdinitramid ADN]  
 Main (potential) use: Oxidizer, component of binary explosives, promising oxidizer for space applications<sup>[41]</sup>, signature-free and environmentally friendly oxidizer<sup>[41]</sup>, replacement for AP<sup>[44]</sup>, possible future solid minimum smoke propellant for tactical missiles or as an underwater explosive<sup>[50]</sup>

Structural formula:



	<b>ADN</b>
Formula	$\text{H}_4\text{N}_4\text{O}_4$
Molecular mass [g mol <sup>-1</sup> ]	124.06
Appearance at RT	Odorless yellowish-white crystalline solid, yellowish-white prills or granules or white powder <sup>[58]</sup>
IS [J]	4 Nm <sup>[17]</sup> , 3–5 Nm <sup>[1,2]</sup> , 3–4 <sup>[3]</sup> , 5 <sup>[4]</sup> , 3.7 <sup>[6]</sup> , 4 (crystals) <sup>[10]</sup> , 4 (prills) <sup>[10]</sup> , $H_{50\%} = 31$ cm (recryst., powder ADN, 2 kg mass, BAM) <sup>[11]</sup> , $H_{50\%} = 59$ cm (prills ~200 µm diameter, 2 kg mass, BAM) <sup>[11]</sup> , 5.0 Nm (as synthesized) <sup>[12]</sup> , 5.0 Nm (after emulsion crystallization) <sup>[12]</sup> , level 1 (aggregation) <sup>[13]</sup> , level 1 (needle-like crystals) <sup>[13]</sup> , level 3 (powder) <sup>[13]</sup> , level 3 (column-like crystals) <sup>[13]</sup> , 102 mm (drop height, 5/10 positive, B.M., 3.6 kg mass, 10 mg sample) <sup>[20]</sup> , 3.7 (BAM, Julius-Peters) <sup>[23]</sup> , 3.5–6.9 cm (ABL, Thiokol prilled ADN unspecified additive added) <sup>[24]</sup> , F of I = 30 (2.3 mL gas evolved) <sup>[25]</sup> , 3.3 <sup>[26]</sup> , 3.5 Nm <sup>[31]</sup> , 16.8 cm (median height, Rotter impact, raw ADN) <sup>[35]</sup> , 73.92 cm (median height, Rotter impact, emulsion-processed ADN) <sup>[35]</sup> , 3 Nm (Eurenc sample) <sup>[36]</sup> , 6 Nm (ADN prills with 1% GUDN) <sup>[36]</sup> , 4 Nm (ADN prills with 0.2% Akardite II) <sup>[36]</sup> , 2.5 (as-received ADN, 99.82% purity, 0.04 wt.% nitrate) <sup>[39]</sup> , 3.2 (as-received ADN, 99.88% purity, 0.02 wt.% nitrate) <sup>[39]</sup> , 2.5–3.2 (prilled ADN, 0.5% Cab-O-Sil added, 99.86% purity, 0.09 wt.% nitrate) <sup>[39]</sup> , 2.0–2.5 (prilled ADN, 0.5% Cab-O-Sil added, 99.76% purity, 0.07 wt.% nitrate) <sup>[39]</sup> , 3.3 (BAM, RT, ADN prills) <sup>[50]</sup>

FS [N]	64 <sup>[17,31]</sup> , 64–72 <sup>[1]</sup> , >350 <sup>[3,6]</sup> , 72 <sup>[4]</sup> , 72 (as synthesized) <sup>[12]</sup> , 72 (after emulsion crystallization) <sup>[12]</sup> , level 6 (aggregation) <sup>[13]</sup> , level 6 (needle-like crystals) <sup>[13]</sup> , level 7 (powder) <sup>[13]</sup> , level 7 (column-like crystals) <sup>[13]</sup> , >360 (limiting load, BAM, 100 mg sample) <sup>[20]</sup> , 11 ± 30 @ 353 N (BAM, Julius-Peters) <sup>[23]</sup> , 420 lb @ 2 feet/s (ABL, Thiokol prilled ADN unspecified additive added) <sup>[24]</sup> , up to 560 lb @ 8 feet/s (ABL, Thiokol prilled ADN unspecified additive added) <sup>[24]</sup> , 360 (BAM) <sup>[25]</sup> , 212 <sup>[26]</sup> , 144 (Eurelco sample) <sup>[36]</sup> , 120 (ADN prills with 1% GUDN) <sup>[36]</sup> , 144 (ADN prills with 0.2% Akardite II) <sup>[36]</sup> , 250 (as-received ADN, 99.82% purity, 0.04 wt.% nitrate) <sup>[39]</sup> , 280–310 (as-received ADN, 99.88% purity, 0.02 wt.% nitrate) <sup>[39]</sup> , ~180 (prilled ADN, 0.5% Cab-O-Sil added, 99.86% purity, 0.09 wt.% nitrate) <sup>[39]</sup> , ~200 (prilled ADN, 0.5% Cab-O-Sil added, 99.76% purity, 0.07 wt.% nitrate) <sup>[39]</sup> , >35 <sup>[41]</sup> , 212 (Julius-Peters, porcelain plate and peg, ADN prills) <sup>[50]</sup> , >35 kp (recryst. ADN, powder, BAM) <sup>[11]</sup> , >35 kp (recryst. ADN, prills ~ 200 µm diameter, BAM) <sup>[11]</sup>
ESD [J]	0.45 <sup>[4,25]</sup> , $E_{50} = 3.5$ (aggregation) <sup>[13]</sup> , $E_{50} = 4.3$ (needle-like crystals) <sup>[13]</sup> , $E_{50} = 2.7$ (powder) <sup>[13]</sup> , $E_{50} = 3.7$ (column-like crystals) <sup>[13]</sup> , >156 mJ (closed container, Franklin Applied Physics app.) <sup>[20]</sup> , >156 mJ (open container, Franklin Applied Physics app.) <sup>[20]</sup> , ≥726 mJ <sup>[23]</sup> , ignition @ 4.5 but not @ 0.45 J (raw ADN) <sup>[35]</sup> , ignition @ 4.5 but not @ 0.45 J (emulsion-processed ADN) <sup>[35]</sup> >156 mJ (crystals, closed) <sup>[10]</sup> , >156 mJ (crystals, open) <sup>[10]</sup> , >156 mJ (prills, closed) <sup>[10]</sup> , >156 mJ (prills, open) <sup>[10]</sup>
N [%]	45.2
Ω [%]	25.8
$T_{\text{phase transitions}}$ [°C]	No phase transition in -150 to +80 °C temperature range <sup>[11]</sup> , 2.0 GPa ( $\alpha$ - $\beta$ phase transition pressure) <sup>[16]</sup> , $\alpha$ - $\beta$ phase transition is reversible <sup>[16]</sup> , $\beta$ -phase converts to $\alpha$ -phase @ $P < \sim 2.0$ GPa <sup>[16]</sup> , $\alpha$ -phase is present @ low pressure ranges <2 GPa and no phase transition occurs below the mpt. <sup>[41]</sup> , $\alpha$ -phase @ $p < 2 \times 10^4$ atm (stable, monoclinic prism crystals) <sup>[56]</sup> , $\beta$ -phase @ $p > 2 \times 10^4$ atm <sup>[56]</sup> Reversible, in crystal <sup>[27]</sup> : $\alpha - \text{ADN} \xrightleftharpoons[2.0 \text{ GPa}]{\text{ }} \beta - \text{ADN}$ (monoclinic)

ADN sample	ADN (% w/w)	Nitrates (% w/w)	Mpt. (°C)	Metals (ppm)	Volatile material (% w/w)	Others (ppm)
Standard	99.5	< 0.1	93	2,500	0.05	25
Flight grade from lab	99.5	< 0.1	93	5	0.05	45
Flight grade from bench scale	99.5	< 0.1	93	5	0.05	5
Flight grade from pilot plant	99.5	< 0.1	93	5	0.05	8

93.1 (as-received ADN, 99.82% purity, 0.04 wt.% nitrate)<sup>[39]</sup>, 93.2 (as-received ADN, 99.88% purity, 0.02 wt.% nitrate)<sup>[39]</sup>, 92.6 (prilled ADN, 0.5% Cab-O-Sil added, 99.86% purity, 0.09 wt.% nitrate)<sup>[39]</sup>, 92.4 (prilled ADN, 0.5% Cab-O-Sil added, 99.76% purity, 0.07 wt.% nitrate)<sup>[39]</sup>, 91.2 (endo, Al-drilled crucibles, DSC @ 5 °C/min, crystalline ADN)<sup>[44]</sup>, 91<sup>[46]</sup>, 92.06 (endo, peak max, DSC)<sup>[45]</sup>

$T_{\text{m.p.}}$ [°C]	<p>91.5<sup>[2,13]</sup>, 93<sup>[4,5,7,39,58]</sup>, 94<sup>[9,18,10,23]</sup>, 91.5<sup>[10]</sup>, 90.7<sup>[10]</sup>, 93.5<sup>[10,41]</sup>, 92<sup>[10]</sup>; 92 (DSC @ 5 K min<sup>-1</sup>, crystals in Al pans)<sup>[10]</sup>, 90 (DSC @ 5 K min<sup>-1</sup>, prills in Al pans)<sup>[10]</sup>, 92 (crystals, TG-DTA-FTIR-MS @ 5 K/min)<sup>[10]</sup>, 90 (prills, TG-DTA-FTIR-MS @ 5 K/min)<sup>[10]</sup>, 91.5–92.5<sup>[12,31]</sup>, 92–95 (depending on the amount of AN impurity present)<sup>[16,56]</sup>, 92.7 (DSC, crude product)<sup>[12]</sup>, 90.4 (DSC, recryst. from paraffin oil emulsion)<sup>[12]</sup>, 95 (DSC @ 2 °C/min)<sup>[16]</sup>, 92.4 (onset, endo), 93.4 (peak max., endo, DSC, raw ADN)<sup>[22]</sup>, 88.9 (onset, endo), 92.7 (peak max., endo) (DSC, ADN from THF)<sup>[22]</sup>, 91.1 (onset, endo), 94.4 (peak max., endo) (DSC, ADN from 1-propanol)<sup>[22]</sup>, 92–94<sup>[24]</sup>, 92–94 (Thiokol prilled ADN unspecified additive added)<sup>[24]</sup>, 365–368 K (<math>\alpha</math>-ADN)<sup>[27]</sup>, 92.7 (peak max., DSC, crude ADN)<sup>[31]</sup>, 90.35 (peak max., DSC, ADN particles from paraffin oil emulsion without additives)<sup>[31]</sup>, 89.9 (peak max., DSC, ADN particles from silicone oil emulsion with stabilizer)<sup>[31]</sup>, 92.04 (onset), 93.21 (peak) (DSC, raw crystalline ADN)<sup>[35]</sup>, 87.91 (onset), 91.12 (peak) (DSC, emulsion processed ADN)<sup>[35]</sup>, 91.01 (endo, onset), 92.97 (endo, peak max.) (DSC, ADN prills tempered @ 70 °C for 5 h)<sup>[36]</sup>, 94.0, 93.8 (DSC, prilled ADN, fluid system prilling process)<sup>[47]</sup>, 93 (ADN prills, DSC @ 10 °C/min, 1.3–1.5 mg sample)<sup>[50]</sup>, 91 (DTA @ 5 °C/min)<sup>[52]</sup>, 92.9<sup>[54]</sup>, 91–93.5 (DSC, NEXPLO sample)<sup>[55]</sup>, 92.5<sup>[56]</sup>, ~92 (observed, @ 15 K/min)<sup>[56]</sup>, 92<sup>[57]</sup>, 93.5 (endo, DSC @ 10 °C/min)<sup>[11]</sup></p> <p>Values from<sup>[38]</sup>:</p> <table border="1"> <thead> <tr> <th>ADN sample</th><th>ADN (% w/w)</th><th>Nitrates (% w/w)</th><th>Mpt. (°C)</th><th>Metals (ppm)</th><th>Volatile material (% w/w)</th><th>Others (ppm)</th></tr> </thead> <tbody> <tr> <td>Standard</td><td>99.5</td><td>&lt; 0.1</td><td>93</td><td>2,500</td><td>0.05</td><td>25</td></tr> <tr> <td>Flight grade from lab</td><td>99.5</td><td>&lt; 0.1</td><td>93</td><td>5</td><td>0.05</td><td>45</td></tr> <tr> <td>Flight grade from bench scale</td><td>99.5</td><td>&lt; 0.1</td><td>93</td><td>5</td><td>0.05</td><td>5</td></tr> <tr> <td>Flight grade from pilot plant</td><td>99.5</td><td>&lt; 0.1</td><td>93</td><td>5</td><td>0.05</td><td>8</td></tr> </tbody> </table> <p>93.1 (as-received ADN, 99.82% purity, 0.04 wt.% nitrate)<sup>[39]</sup>, 93.2 (as-received ADN, 99.88% purity, 0.02 wt.% nitrate)<sup>[39]</sup>, 92.6 (prilled ADN, 0.5% Cab-O-Sil added, 99.86% purity, 0.09 wt.% nitrate)<sup>[39]</sup>, 92.4 (prilled ADN, 0.5% Cab-O-Sil added, 99.76% purity, 0.07 wt.% nitrate)<sup>[39]</sup>, 91.2 (endo, Al-drilled crucibles, DSC @ 5 °C/min, crystalline ADN)<sup>[44]</sup>, 91<sup>[46]</sup>, 92.06 (endo, peak max, DSC)<sup>[45]</sup></p>	ADN sample	ADN (% w/w)	Nitrates (% w/w)	Mpt. (°C)	Metals (ppm)	Volatile material (% w/w)	Others (ppm)	Standard	99.5	< 0.1	93	2,500	0.05	25	Flight grade from lab	99.5	< 0.1	93	5	0.05	45	Flight grade from bench scale	99.5	< 0.1	93	5	0.05	5	Flight grade from pilot plant	99.5	< 0.1	93	5	0.05	8
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1	172																				
1.5	176																				
2	179																				
2.5	181																				
$T_{\text{b.p.}}$ [°C]	Dec. above 135 °C, no b.p. observed <sup>[58]</sup>																				
$T_{\text{dec}}$ [°C]	127 (dec. energy = $255 \pm 12.5$ kJ/mol) <sup>[2,31]</sup> , 134 <sup>[7]</sup> (autoignition temperature = 160 °C) <sup>[4]</sup> , 189 <sup>[9]</sup> , 189, 127, 183, 190, 130 <sup>[10]</sup> , 127 (DSC @ 5 K min <sup>-1</sup> , crystals in sealed glass ampoules) <sup>[10]</sup> , 133 (DSC @ 5 K min <sup>-1</sup> , prills in sealed glass ampoules) <sup>[10]</sup> , 145.3 (onset, exo), 184.2 (peak max., exo) (DSC, raw ADN) <sup>[22]</sup> , 152.2 (onset, exo), 183.3 (peak max., exo) (DSC, ADN from THF) <sup>[22]</sup> , 159.1 (onset, exo), 176.0 (peak max., exo) (DSC, ADN from 1-propanol) <sup>[22]</sup> , 160 (onset, DSC @ 20 °C/min) <sup>[24]</sup> , 180 (onset, DSC @ 20 °C/min, Thiokol prilled ADN unspecified additive added) <sup>[24]</sup> , 126.8 (onset), 159.3 (peak max., DSC, crude ADN) <sup>[31]</sup> , 146.9 (onset), 176.5 (peak max., DSC, ADN particles from paraffin oil emulsion without additives) <sup>[31]</sup> , 145.24 (onset), 173.4 (peak max., DSC, ADN particles from silicone oil emulsion with stabilizer) <sup>[31]</sup> , 151.86 (onset), 191.30 (peak) (DSC, raw crystalline ADN) <sup>[35]</sup> , 167.46 (onset), 188.17 (peak) (DSC, emulsion-processed ADN) <sup>[35]</sup> , 152.65 (exo, onset), 185.65 (exo, peak max.) (DSC, ADN prills tempered @ 70 °C for 5 h) <sup>[36]</sup> , 182.9 (onset, exo), 257.5 (exo peak max.) (Al-drilled crucibles, DSC @ 5 °C/min, crystalline ADN) <sup>[44]</sup> , 183.7 (onset), 248.2 (peak max., 80.9% mass loss, TG @ 5 °C/min, crystalline ADN) <sup>[44]</sup> , 182.7 (exo, peak max., DSC) <sup>[45]</sup> , 155 (ADN prills, DSC @ 10 °C/min, 1.3–1.5 mg sample) <sup>[50]</sup> , 135–220 (single step dec., TG @ 5 °C/min) <sup>[52]</sup> , 150 (onset exotherm), 230 (end of exotherm) (DSC, NEXPLO sample) <sup>[55]</sup> , 120–140 @ 2.0–10.0 GPa ( $\beta$ -ADN undergoes dec. forming AN and $N_2O$ ) <sup>[56]</sup> , 190.1 (exo peak max., DSC @ 10 °C/min) <sup>[11]</sup>																				
	TGA, various heating rates <sup>[45]</sup> :																				
	<table border="1"> <thead> <tr> <th>Heating rate (°C/min)</th><th>Dec. onset <math>T</math> (°C)</th><th>Dec. <math>T</math> (°C)</th><th>Dec. final <math>T</math> (°C)</th></tr> </thead> <tbody> <tr> <td>1</td><td>132</td><td>172</td><td>197</td></tr> <tr> <td>1.5</td><td>134</td><td>174</td><td>210</td></tr> <tr> <td>2</td><td>135</td><td>175</td><td>220</td></tr> <tr> <td>2.5</td><td>135</td><td>176</td><td>230</td></tr> </tbody> </table>	Heating rate (°C/min)	Dec. onset $T$ (°C)	Dec. $T$ (°C)	Dec. final $T$ (°C)	1	132	172	197	1.5	134	174	210	2	135	175	220	2.5	135	176	230
Heating rate (°C/min)	Dec. onset $T$ (°C)	Dec. $T$ (°C)	Dec. final $T$ (°C)																		
1	132	172	197																		
1.5	134	174	210																		
2	135	175	220																		
2.5	135	176	230																		
	Summary of literature values ( $T_{\text{exo}}$ = exothermic peak, $T_{\text{decomp}}$ = onset of thermal dec.): DSC thermal analysis with different heating rates (modulated DSC method = expt. carried out with linear heating rate of 0.5 K/min superimposed by a sinusoidal temperature variation to improve resolution and to enhance the sensitivity of the DSC) <sup>[56]</sup> :																				

	$dT/dt$ (K/min)	$T_{dec.}$ (°C)	$T_{exo}$ (°C)
	5	150	180
	5	150	180.3
	10	154.4	198
	10	150	190
	15 (DTA)	160	190
	20	150	189
	0.5 (modulated DSC)	126.8	159.3

DSC @ 10 °C/min<sup>[60]</sup>:

Sample type	Dec. onset $T$ (°C)	Max. peak $T$ (°C)
Pristine ADN	177	193
Prilled, PS, 5 wt.%	181	186
Prilled HTPB, 5 wt.%	170	190
Sonicated, PS, 5 wt.%	171	192
Sonicated, HTPB, 5 wt.%	178	181
Sonicated, HTPB, 20 wt.%	196	198
Pristine ADN	126	159
Prilled ADN	168	195

$\rho$  [g cm<sup>-3</sup>]

1.812 (@ 298 K), 1.8183<sup>[3]</sup>, 1.81 (@ 25 °C)<sup>[4,6,50]</sup>, 1.56 (liq., @ 100 °C)<sup>[4]</sup>, 1.82–1.84<sup>[12,31,56]</sup>, 1.660 (pure ADN, cast, ambient pressure, 92% TMD)<sup>[21]</sup>, 1.640 (pure ADN cast, vacuum, 90% TMD)<sup>[21]</sup>, 1.580 (pure ADN, pressed, 80 MPa, 25 mm diameter, 87% TMD)<sup>[21]</sup>, 1.660 (pure ADN, pressed, 80 MPa, 40 mm diameter, 92% TMD)<sup>[21]</sup>, 1.670 (pure ADN, pressed, 90 MPa, 10 mm diameter, 93% TMD)<sup>[21]</sup>, 1.560 (liq. @ 100 °C)<sup>[21]</sup>, 1.81<sup>[23,39,58]</sup>, 1.60–1.84 ( $\rho_{p,ADN}$  (s))<sup>[28]</sup>, 1.55 ( $\rho_{p,ADN}$  (l))<sup>[28]</sup>, 1.82 (as-received ADN, 99.82% purity, 0.04 wt.% nitrate)<sup>[39]</sup>, 1.81 (as-received ADN, 99.88% purity, 0.02 wt.% nitrate)<sup>[39]</sup>, 1.80 (prilled ADN, 0.5% Cab-O-Sil added, 99.86% purity, 0.09 wt.% nitrate)<sup>[39]</sup>, 1.79 (prilled ADN, 0.5% Cab-O-Sil added, 99.76% purity, 0.07 wt.% nitrate)<sup>[39]</sup>, 1.8184 ( $P_2$ <sub>1</sub>/c crystal)<sup>[41]</sup>, 1.820 (@ 25 °C, X-ray measured, NEXPLO sample)<sup>[55]</sup>, 1.560 (pycnometer, liquid @ 100 °C, NEXPLO sample)<sup>[55]</sup>, 1.660 (92% TMD, NEXPLO sample, cast, ambient pressure)<sup>[55]</sup>, 1.640 (90% TMD, NEXPLO sample, vacuum cast)<sup>[55]</sup>, 1.760 (97% TMD, NEXPLO ADN/MgO (99/1), cast, ambient pressure)<sup>[55]</sup>, 1.740 (95% TMD, NEXPLO ADN/MgO (99/1), vacuum cast)<sup>[55]</sup>, 1.580 (87% TMD, NEXPLO sample, pressed, 80 MPa, 25 mm diameter)<sup>[55]</sup>, 1.660 (92% TMD, NEXPLO sample, pressed, 80 MPa, 40 mm diameter)<sup>[55]</sup>, 1.670 (93% TMD, NEXPLO sample, pressed, 90 MPa, 10 mm diameter)<sup>[55]</sup>, 1.8 (crystal)<sup>[56]</sup>, 1.801 (X-ray)<sup>[56]</sup>, 1.8139(2) (bulk  $\rho$  @ RT, powder XRD)<sup>[11]</sup>, 1.8183(10) (bulk  $\rho$ , single-crystal XRD @ 293 K)<sup>[11]</sup>

$\rho$  measurements of raw and stabilized ADN samples<sup>[37]</sup>:

Sample	$\rho$ @ 20 °C (g cm <sup>-3</sup> )	Sample	$\rho$ @ 20 °C (g cm <sup>-3</sup> )
Raw ADN (Eureenco sample)	1.793	ADN + 0.5% AKII (batch process)	1.794
ADN prills without stabilizer	1.726 (visible gas bubbles)	ADN + 0.5% Sx (batch process)	1.792
ADN prills without stabilizer	1.788	ADN + 0.5% Sx (continuous attempt)	1.805
ADN + 0.5% MgO (batch process)	1.755 (agglomeration)	ADN + 0.5% Sx (continuous attempt)	1.797

0.84 (bulk  $\rho$ , as-received ADN, 99.82% purity, 0.04 wt.% nitrate)<sup>[39]</sup>, 0.89 (bulk  $\rho$ , as-received ADN, 99.88% purity, 0.02 wt.% nitrate)<sup>[39]</sup>, 1.10 (bulk  $\rho$ , prilled ADN, 0.5% Cab-O-Sil added, 99.86% purity, 0.09 wt.% nitrate)<sup>[39]</sup>, 1.12 (bulk  $\rho$ , prilled ADN, 0.5% Cab-O-Sil added, 99.76% purity, 0.07 wt.% nitrate)<sup>[39]</sup>

ADN particles milled in *n*-decane using a diving basket mill filled with ceramic beads, with Aerosil® added as anticaking agent (microstructure analysis using Rietveld, X-ray diffraction)<sup>[51]</sup>:

Sample	Crystal size Length (nm)	Volume (Å <sup>3</sup> )	$\rho$ (g cm <sup>-3</sup> )
ADN reference	379	455.1	1.810
ADN-decane, roughly ground	1,532	456.6	1.805
ADN-decane, finely ground	723	457.0	1.803
ADN fine, washed and dried	162	457.2	1.802

Density versus temperature for ADN, approx. values from graph<sup>[11]</sup>:

T (K)	$\rho$ (g cm <sup>-3</sup> )	T (K)	$\rho$ (g cm <sup>-3</sup> )
120	1.866	250	1.834
150	1.86	275	1.825
175	1.856	295	1.82
190	1.852	335	1.805
210	1.845	344	1.802
235	1.838		

Heat of formation	<p>-125.3 kJ/mol (formation energy)<sup>[1]</sup>, -1,209 kJ/kg (<math>\Delta H_f^\circ</math>)<sup>[5]</sup>, 150.6 kJ mol<sup>-1</sup>(<math>\Delta H_f^\circ</math>)<sup>[31]</sup>, -1,207 kJ/kg (ICT thermochemical database)<sup>[32]</sup>, -32.16 kcal/mol (<math>\Delta H_f^\circ</math>)<sup>[33]</sup>, -148 kJ/mol (<math>\Delta H_f^\circ</math>)<sup>[46]</sup>, -1,207.5 J/g (<math>\Delta H_f^\circ</math>, ICT thermochemical database)<sup>[54]</sup>, -149.8 kJ/mol (<math>\Delta H_f^\circ</math>, ICT thermochemical database)<sup>[54]</sup>, -35.4 kcal mol<sup>-1</sup><sup>[4]</sup>, -150.6 kJ mol<sup>-1</sup><sup>[12]</sup>, -148 kJ/mol<sup>[39]</sup>, -256.3 kcal/kg (<math>\Delta H_f^\circ</math>, 298 K)<sup>[56]</sup>, -35.8 kcal/mol (enthalpy of form.)<sup>[56]</sup>, -150 kJ/mol (enthalpy of form.)<sup>[6, 23, 58]</sup>, <math>32.16 \pm 0.11</math> kcal/mol (enthalpy of form.)<sup>[53]</sup>, -150.2 kJ/mol (<math>\Delta H_f^\circ</math>, exptl.)<sup>[59]</sup>, -123.0 kJ/mol (<math>\Delta H_f^\circ</math>, calcd., Born–Haber cycles)<sup>[59]</sup>, -149 kJ/mol (<math>\Delta H_f</math> @ constant vol., exptl. bomb calorimeter, 1.46061 g sample)<sup>[11]</sup>, -151 kJ/mol (<math>\Delta H_f</math> @ constant vol., exptl. bomb calorimeter, 0.9771 g sample)<sup>[11]</sup>, -150 kJ/mol (<math>\Delta H_f</math> @ constant vol., exptl. bomb calorimeter, 1.2836 g sample)<sup>[11]</sup>, -146 kJ/mol (<math>\Delta H_f</math> @ constant vol., exptl. bomb calorimeter, 1.3284 g sample)<sup>[11]</sup>, -144 kJ/mol (<math>\Delta H_f</math> @ constant vol., exptl. bomb calorimeter, 1.4017 g sample)<sup>[11]</sup>, -148 ± 10 kJ/mol (<math>\Delta H_f</math> (average value) @ constant vol., exptl. bomb calorimeter)<sup>[11]</sup></p>		
Heat of combustion	<p>+101.3 kcal/mol<sup>[4]</sup>, 424 kJ/mol<sup>[39]</sup>, -35.8 kcal/mol<sup>[56]</sup>, 979.45 kJ/mol (exptl. bomb calorimeter, 1.46061 g sample)<sup>[11]</sup>, 977.745 kJ/mol (exptl. bomb calorimeter, 0.9771 g sample)<sup>[11]</sup>, 978.566 kJ/mol (exptl. bomb calorimeter, 1.2836 g sample)<sup>[11]</sup>, 982.824 kJ/mol (exptl. bomb calorimeter, 1.3284 g sample)<sup>[11]</sup>, 984.450 kJ/mol (exptl. bomb calorimeter, 1.4017 g sample)<sup>[11]</sup></p>		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^\circ [\text{kJ kg}^{-1}]$	2,784	<p>3,337 [H<sub>2</sub>O (l) @ 25 °C] (calcd., ICT thermodynamic code)<sup>[9,32,34]</sup></p> <p>2,668 J/g [H<sub>2</sub>O (g)]<sup>[34]</sup></p> <p>3,337 [H<sub>2</sub>O (g)] (calcd., ICT thermodynamic code)<sup>[54]</sup></p> <p>3,096 (@ 1.840 g cm<sup>-3</sup>, Q, calcd.)<sup>[5]</sup></p>	
$T_{\text{ex}}$ [K]	2,319	2,514 (calcd., ICT code) <sup>[32]</sup>	
$p_{\text{C,J}}$ [kbar]	270	<p>21 GPa (calcd., CHEETAH 2.0 with BKW EOS and BKWS product library)<sup>[21]</sup></p> <p>92.6 MPa (calcd., ICT code)<sup>[32]</sup></p> <p>2.5 GPa (@ 1.840 g cm<sup>-3</sup>, calcd.)<sup>[5]</sup></p>	

VoD [ $\text{m s}^{-1}$ ]	8,502	7.62 mm/ $\mu\text{s}$ (@ 1.72 g $\text{cm}^{-3}$ and heat of formation of -135.0 kJ $\text{mol}^{-1}$ , calcd., CHEETAH 2.0 with BKW EOS and BKWS product library) <sup>[21]</sup> 6,480 (@ 1.840 g $\text{cm}^{-3}$ , calcd.) <sup>[5]</sup>	~7,000 <sup>[4]</sup> No det. (@ 1.72 g $\text{cm}^{-3}$ , 25 mm charge diameter, thin-walled PMMA cylinders) <sup>[21]</sup>  4.3 mm/ $\mu\text{s}$ (@ 1.72 g $\text{cm}^{-3}$ , 40 mm charge diameter, thin-walled PMMA cylinders) <sup>[21]</sup>  5.4 mm/ $\mu\text{s}$ (@ 1.72 g $\text{cm}^{-3}$ , 60 mm charge diameter, thin-walled PMMA cylinders) <sup>[21]</sup>  6.0 mm/ $\mu\text{s}$ (@ 1.72 g $\text{cm}^{-3}$ , 100 mm charge diameter, thin-walled PMMA cylinders) <sup>[21]</sup>
$V_0$ [ $\text{L kg}^{-1}$ ]	984	592 (calcd., ICT thermodynamic code) <sup>[9]</sup>  592 (@ 25 °C) <sup>[34]</sup>  592 (thermodynamically controlled combustion @ 25 °C without water, calcd., ICT thermodynamic code) <sup>[54]</sup>	1,084 <sup>[8]</sup>
Critical diameter [cm]		40 mm <sup>[55]</sup> , between 25 and 40 mm <sup>[21]</sup>	
Critical pressure of explosion initiation by impact [GPa]		$p_{\text{cr}} = 0.57 \pm 0.01$ GPa (polycryst. ADN) <sup>[42,43]</sup> ; $\sigma_{\text{ult}} = 86$ MPa (polycryst. ADN) <sup>[42,43]</sup>	
Specific impulse ( $I_{\text{sp}}$ ) [s]		254 (formulations containing 30% GAP-based binder, calcd.) <sup>[26]</sup>	
5 s explosion $T$ [°C] Ignition $T$ [°C]		194 (aggregation) <sup>[22]</sup> , 220 (needle-like crystals) <sup>[13]</sup> , 202 (powder) <sup>[13]</sup> , 194 (column-like crystals) <sup>[13]</sup> , 160 <sup>[19]</sup> , 142 <sup>[25]</sup> , 147.7 (emulsion-processed ADN) <sup>[35]</sup>	
100 °C heat test [% mass loss]		4% mass loss/24 h @ 100 °C <sup>[12,31]</sup>	

Thermal stability [moles gas per mole ADN/no. h]	<p>@ 120 °C: 1.25/22, 1.45/72, 2.53/561<sup>[18]</sup>  @ 220 °C: 2.13/22, 2.2/72<sup>[18]</sup>  @ 320 °C: 2.4/22, 2.3/72<sup>[18]</sup></p> <p>2.1–5.7% mass loss @ 80 °C, 20 days (Eureenco sample)<sup>[36]</sup>,  0.36% mass loss @ 80 °C (ADN prills with 1% GUDN)<sup>[36]</sup>,  0.20% mass loss @ 80 °C (ADN prills with 0.2% Akardite II)<sup>[36]</sup></p> <p>Approximate mass loss (%) of unstabilized ADN-ICT @ 65–80 °C over time (days)<sup>[49]</sup>:</p> <table border="1"> <thead> <tr> <th rowspan="2">Time (days)</th><th colspan="4">Temperature (°C)</th></tr> <tr> <th>65</th><th>70</th><th>75</th><th>80</th></tr> </thead> <tbody> <tr><td>25</td><td>0.05</td><td>0.05</td><td>0.1</td><td>0.3</td></tr> <tr><td>50</td><td>0.1</td><td>0.1</td><td>0.25</td><td>3.0</td></tr> <tr><td>75</td><td>0.1</td><td>0.2</td><td>0.55</td><td></td></tr> <tr><td>100</td><td>0.1</td><td>0.2</td><td>0.8</td><td></td></tr> <tr><td>125</td><td>0.2</td><td>0.25</td><td>1.6</td><td></td></tr> <tr><td>150</td><td>0.25</td><td>0.45</td><td>3.4</td><td></td></tr> <tr><td>175</td><td>0.2</td><td>0.6</td><td></td><td></td></tr> <tr><td>200</td><td>0.2</td><td>0.7</td><td></td><td></td></tr> <tr><td>225</td><td>0.25</td><td>0.75</td><td></td><td></td></tr> <tr><td>250</td><td>0.25</td><td>0.9</td><td></td><td></td></tr> <tr><td>300</td><td>0.25</td><td>1.1</td><td></td><td></td></tr> <tr><td>325</td><td>0.2</td><td>1.25</td><td></td><td></td></tr> <tr><td>350</td><td></td><td>1.5</td><td></td><td></td></tr> </tbody> </table> <p>Molten ADN is unstable without a stabilizer and may cause an ignition due to autocatalytic decomposition<sup>[55]</sup></p>	Time (days)	Temperature (°C)				65	70	75	80	25	0.05	0.05	0.1	0.3	50	0.1	0.1	0.25	3.0	75	0.1	0.2	0.55		100	0.1	0.2	0.8		125	0.2	0.25	1.6		150	0.25	0.45	3.4		175	0.2	0.6			200	0.2	0.7			225	0.25	0.75			250	0.25	0.9			300	0.25	1.1			325	0.2	1.25			350		1.5		
Time (days)	Temperature (°C)																																																																										
	65	70	75	80																																																																							
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Vacuum stability test [cm <sup>3</sup> /h]	0.09% mass loss @ 50 °C (duration not specified) <sup>[20]</sup> , 0.73 mL/5 g @ 80 °C/40 h <sup>[25]</sup> , 1.75–14.68 mL (converted to 100 °C, 40 h, 1.0 g Eureenco sample) <sup>[36]</sup> , 0.68 mL (converted to 100 °C, 40 h, 1.0 g ADN prills with 1% GUDN) <sup>[36]</sup> , 0.47 mL (converted to 100 °C, 40 h, 1.0 g ADN prills with 0.2% Akardite II) <sup>[36]</sup>																																																																										

	VST and mass loss of different samples <sup>[48]</sup> :		
	Sample	VST recalculated to 100 °C, 40 h (mL/g)	Mass loss @ 80 °C, 20 days (%)
	Raw ADN (Eureno)	1.75–14.68	2.1–5.7
	Raw ADN (Eureno)	5.47	1.8
	Mixed batches ADNP 51 fine prills	1.30	0.3
	Mixed batches ADNP 51 fine prills	1.14	1.2
	Stabilized ADN prills, 169 µm	0.14	0.1
	Stabilized ADN prills, 48 µm	0.43	0.9
Vapor pressure [atm @ °C]	$1.71 \times 10^{-12}$ mm Hg (solid) <sup>[57]</sup>		
$C_p$ [cal/g/K]	$2.094 \times 10^{-1} + 3.361 \times 10^{-4}T^{[28]}$ , 0.59 <sup>[28]</sup> , $1.26 \times 10^3$ J/kg/K <sup>[28]</sup> , 0.49 <sup>[28]</sup>		
Specific heat ( $C_p$ ) [J kg <sup>-1</sup> K <sup>-1</sup> ]	$1,697 \pm 8\%$ (solid) <sup>[44]</sup> , $2,195 \pm 5\%$ (liquid) <sup>[44]</sup>		
Heat capacity, $C_p$ [J/g]	$1.8^{[4]}$ , $1.8 \pm 0.2$ (DSC, solid, NEXPLO sample) <sup>[55]</sup> , $1.77 \text{ kJ}/(\text{kg K})^{[55]}$ , $1.8 \pm 0.2$ (solid) <sup>[21]</sup>		
Thermal conductivity, $\lambda$ [J m <sup>-1</sup> K <sup>-1</sup> s <sup>-1</sup> ]	$0.653^{[44]}$		
Coefficient of thermal expansion	$1.91 \times 10^{-4}$ 1/K (gas pycnometer, volumetric, solid, NEXPLO sample) <sup>[55]</sup>		
Thermal diffusivity, $D_{th}$ [m <sup>2</sup> s <sup>-1</sup> ]	$1.912 \times 10^{-7} \pm 6\%^{[44]}$		
Burn rate [mm/s]	Dependence of burn rate on pressure (5 mm sample diameter) <sup>[29]</sup> :		
	$p$ (MPa)	$v \times 10^2$ (m/s)	$p$ (MPa)
	0	~0.4	6
	2	~1.8	8
	4	~2.0	10
	Dependence of burn rate on pressure (7 mm sample diameter) <sup>[29]</sup> :		
	$p$ (MPa)	$v \times 10^2$ (m/s)	$p$ (MPa)
	0	~0.4	6
	2	~1.8	8
	4	~2.6	10

	<p>Characteristics of ADN combustion (burn rate = <math>v \times 10^2</math>, burning surface temperature = <math>T_s</math>):<sup>[29]</sup></p> <table border="1"> <thead> <tr> <th><math>p</math> (MPa)</th><th><math>v \times 10^2</math> (m/s) (exptl.)</th><th><math>T_s</math> (K) (exptl.)</th></tr> </thead> <tbody> <tr> <td>0.1</td><td>0.27</td><td>560</td></tr> <tr> <td>2</td><td>1.82</td><td>700</td></tr> </tbody> </table> <p>Burn rate &lt;100 atm is higher than that of CL-20, HNF, HMX, RDX, AP, AN, GAP and BAMO,<sup>[56]</sup> with increasing particle size the burn rate of ADN-based propellants increases<sup>[56]</sup>, <math>r_b = 3.5\text{--}11</math> mm/s @ 1–3 atm, ADN pellets burn nonluminously<sup>[56]</sup>, laser-assisted combustion of ADN pellets @ 3 atm produced an unstable flame with only weak dependence on the laser heat flux intensity, whereas @ 5–6 atm pure ADN pellets burned steadily and luminously and stable combustion of pure ADN occurs first at 5–20 atm<sup>[56]</sup>, 20–100 atm is region of unstable combustion where burning is irregular<sup>[56]</sup>, @ high pressures &gt;100 atm stable combustion observed<sup>[56]</sup>, addition of 0.2% of paraffin did not change the burning behavior at low (0.2–20 atm) and high (&gt;100 atm) pressures, but stabilized combustion in 20–100 atm range<sup>[56]</sup>, burning rate of ADN is very sensitive to its preconditioned temperature<sup>[56]</sup>, burning rate of pure ADN shows relatively high pressure sensitivity<sup>[56]</sup></p>	$p$ (MPa)	$v \times 10^2$ (m/s) (exptl.)	$T_s$ (K) (exptl.)	0.1	0.27	560	2	1.82	700
$p$ (MPa)	$v \times 10^2$ (m/s) (exptl.)	$T_s$ (K) (exptl.)								
0.1	0.27	560								
2	1.82	700								
Solubility [g/mL]	<p>Very soluble in <math>\text{H}_2\text{O}</math><sup>[24]</sup>, very soluble in <math>\text{H}_2\text{O}</math> (Thiokol prilled ADN unspecified additive added)<sup>[24]</sup>, 357 g dissolves in 100 g <math>\text{H}_2\text{O}</math> @ 20 °C<sup>[4]</sup>, 0.18 g dissolves in 100 g butyl acetate @ 20 °C<sup>[4]</sup>, 0.003 g dissolves in 100 g <math>\text{CH}_2\text{Cl}_2</math> @ 20 °C<sup>[4]</sup>, 357 g dissolves in 100 g <math>\text{H}_2\text{O}</math><sup>[39]</sup>, 86.9 g dissolves in 100 g <math>\text{MeOH}</math><sup>[39]</sup>, 0.18 g dissolves in 100 g butyl acetate<sup>[39]</sup>, 0.005 g dissolves in 100 g <i>n</i>-heptane<sup>[39]</sup>, 0.003 g dissolves in 100 g dichloromethane<sup>[39]</sup>, 69.8% solubility in <math>\text{H}_2\text{O}</math> @ 0 °C<sup>[46]</sup>, 500,000 mg/L in <math>\text{H}_2\text{O}</math><sup>[57]</sup></p> <p>Crystal types obtained from various solvents<sup>[22]</sup>: propylene carbonate, needle shaped<sup>[22]</sup>; 1-propanol, needle shaped<sup>[22]</sup>; 1-pentanol, needle shaped<sup>[22]</sup>; 1-octanol, needle shaped<sup>[22]</sup>; benzyl alcohol, short, compact needles<sup>[22]</sup>; 2-methyl-2-pentanol, needle shaped<sup>[22]</sup>; ethylene glycol, needle shaped<sup>[22]</sup>; <i>n</i>-butyl acetate, short needles<sup>[22]</sup>; <math>\gamma</math>-butyrolactone, long needles<sup>[22]</sup>; diethylene glycol monoethyl ether, needle shaped<sup>[22]</sup></p>									

	<p>Approximate concentration of ADN @ 40 °C      (g ADN/g solvent): 0.17 propylene carbonate<sup>[22]</sup>, 0.10 1-propanol<sup>[22]</sup>, 0.03 1-pentanol<sup>[22]</sup>, 0.01 1-octanol<sup>[22]</sup>, 0.05 benzyl alcohol<sup>[22]</sup>, 0.03 2-methyl-2-pentanol<sup>[22]</sup>, 0.19 ethylene glycol<sup>[22]</sup>, 1.3 2-propanol<sup>[22]</sup>, 0.05 methyl acetate<sup>[22]</sup>, 0.03 ethyl acetate<sup>[22]</sup>, 0.02 <i>n</i>-butyl acetate<sup>[22]</sup>, 0.19 γ-butyrolactone<sup>[22]</sup>, 0.21 diethylene glycol monoethyl ether<sup>[22]</sup>, 0.01 5-nonenone<sup>[22]</sup>, 0.41 cyclohexanone<sup>[22]</sup>, 0.0 toluene<sup>[22]</sup>, 0.73 triethylamine<sup>[22]</sup>, 0.2 DMSO<sup>[22]</sup>, 0.27 <i>N,N</i>-DMF<sup>[22]</sup>, 0.28 acetonitrile<sup>[22]</sup>, 0.17 acetone<sup>[22]</sup>, 0.26 MeOH<sup>[22]</sup>, 0.28 EtOH<sup>[22]</sup>, 0.28 ethyl methyl ketone<sup>[22]</sup>, 0.27 THF<sup>[22]</sup>, 0.0 trichloromethane<sup>[22]</sup>, 0.0 1,2-dichlorobenzene<sup>[22]</sup>, 0.01 benzonitrile<sup>[22]</sup>, 0.0 diethyl carbonate<sup>[22]</sup>, 0.21 propionaldehyde<sup>[22]</sup>, 0.0 1,2-dichloroethane<sup>[22]</sup>, 0.23 <i>tert</i>-butanol<sup>[22]</sup>, 0.0 chlorobenzene<sup>[22]</sup>, 0.8 (soln.) triethylene glycol<sup>[22]</sup>, 0.05 acetic anhydride<sup>[22]</sup>, 0.23 <i>N</i>-methyl-2-pyrrolidinone<sup>[22]</sup>, 0.8 (soln.) diethylene glycol<sup>[22]</sup></p>																					
Hygroscopicity	<p>Hygroscopic<sup>[24]</sup>, not hygroscopic (Thiokol prilled ADN unspecified additive added)<sup>[24]</sup>, critical RH = 55.2<sup>[4]</sup>      H<sub>2</sub>O content: 0.42% after synthesis<sup>[31]</sup>, 0.41% after emulsion crystallization<sup>[31]</sup>, critical RH = 55.2% @ 25 °C<sup>[39]</sup>, block of ADN standing in air of 50% rel. humidity for a few hours becomes deliquescent on surface<sup>[55]</sup></p> <p>Water absorption test (0.3–0.5 g, enclosed environment with uniform airflow rate of 5 L/min, chamber humidity = 65 ± 2% RH) approx. values from graph<sup>[60]</sup>:</p> <table border="1"> <thead> <tr> <th>Sample</th> <th>Mass gain (%) of sample after 120 min</th> <th>Mass gain (%) of sample after 240 min</th> </tr> </thead> <tbody> <tr> <td>Pristine ADN</td> <td>58</td> <td>70</td> </tr> <tr> <td>Prilled ADN, HTPB coated, 5 wt. %</td> <td>20</td> <td>22</td> </tr> <tr> <td>Sonicated ADN, HTPB coated, 5 wt. %</td> <td>10</td> <td>30</td> </tr> <tr> <td>Prilled ADN, PS coated, 5 wt. %</td> <td>18</td> <td>20</td> </tr> <tr> <td>Sonicated ADN, PS coated, 5 wt. %</td> <td>18</td> <td>32</td> </tr> <tr> <td>Sonicated ADN, PS coated, 5 wt. %, with graphene</td> <td>10</td> <td>16</td> </tr> </tbody> </table>	Sample	Mass gain (%) of sample after 120 min	Mass gain (%) of sample after 240 min	Pristine ADN	58	70	Prilled ADN, HTPB coated, 5 wt. %	20	22	Sonicated ADN, HTPB coated, 5 wt. %	10	30	Prilled ADN, PS coated, 5 wt. %	18	20	Sonicated ADN, PS coated, 5 wt. %	18	32	Sonicated ADN, PS coated, 5 wt. %, with graphene	10	16
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Photosensitivity	Sensitive to light <sup>[24]</sup> , light sensitive (Thiokol prilled ADN unspecified additive added) <sup>[24]</sup> , highly sensitive to sunlight (UV radiation) and should not be exposed to direct sunlight <sup>[55]</sup> , aqueous ADN solns. are sensitive to light <sup>[56]</sup>
Compatibility	Molten ADN is unstable without a stabilizer and may cause an ignition due to autocatalytic decomposition <sup>[55]</sup> , incompatible with many common materials as well as impurities <sup>[55]</sup> , compatible with stainless steel (SS2343, V4A, AISI316), Al, Mg, Au, PTFE, perfluorinated rubber (Viton), polyethylene without dyestuffs, RDX, HMX, zinc oxide, magnesium oxide, Dow Sylgard 170 two-component silicone resin, Plexiglas (as thoroughly cured polymer) <sup>[55]</sup> , incompatible with rust, iron, nickel, copper and its alloys or compounds, silver and its alloys or compounds, cyanoacrylate glue and polyacetal (Delrin) <sup>[55]</sup> , addition of aqueous nitric acid to molten ADN accelerates dec. <sup>[56]</sup> , accelerated dec. in strong acids such as sulfuric acid or nitric acid @ RT since acid-catalytic dec. is proportional to acidity <sup>[56]</sup> , NO <sub>2</sub> (g) accelerates dec. <sup>[56]</sup> , hexamethylenamine, 2-nitrodiphenylamine, methyldiphenylurea, cyanoquanidine and prophosphatane compounds improve ADN thermal stability <sup>[56]</sup> , addition of hexamine increases the FS <sup>[56]</sup>
Particle dimensions	Long needles <sup>[24]</sup> , spheres (Thiokol prilled ADN unspecified additive added) <sup>[24]</sup>
$I_{sp}$ [Ns/kg]	1,986 <sup>[34]</sup>
$I_v$ [Ns/dm <sup>3</sup> ]	3,599 <sup>[34]</sup>
Enthalpy of melting [J/g]	140.3 (as-received ADN, 99.82% purity, 0.04 wt.% nitrate) <sup>[39]</sup> , 141.9 (as-received ADN, 99.88% purity, 0.02 wt.% nitrate) <sup>[39]</sup> , 140.0 (prilled ADN, 0.5% Cab-O-Sil added, 99.86% purity, 0.09 wt.% nitrate) <sup>[39]</sup> , 136.3 (prilled ADN, 0.5% Cab-O-Sil added, 99.76% purity, 0.07 wt.% nitrate) <sup>[39]</sup> , $\Delta H_m = 140 \text{ J/g}$ <sup>[46]</sup>
Surface tension [mN/m]	89 (molten ADN @ 97 °C, measured) <sup>[40]</sup>
$\Delta H_{melt}$ [kJ/kg]	146 (DSC @ 10 °C/min), 1.3–1.5 mg sample, ADN prills <sup>[50]</sup>
Heat of fusion [kJ/kg]	130 ± 5 (DSC, NEXPLO sample) <sup>[55]</sup> , 130 ± 5 <sup>[21]</sup>

Activation energy of thermal dec. [kJ/mol]	101.8 (MKN method) <sup>[52]</sup> Values cited in <sup>[56]</sup> :																				
	<table border="1"> <thead> <tr> <th>Exptl. conditions</th><th><math>E_a</math> (kcal/mol)</th></tr> </thead> <tbody> <tr> <td>DSC (N<sub>2</sub>)</td><td>41.9</td></tr> <tr> <td>DSC (He)</td><td>43.1</td></tr> <tr> <td>DSC (sealed pan)</td><td>30.8</td></tr> <tr> <td>DSC (<math>p = 37.42</math> atm, air)</td><td>29.3</td></tr> <tr> <td>DSC (<math>p = 37.42</math> atm, He)</td><td>29.5</td></tr> <tr> <td>DSC (vacuum, 35 mm Hg)</td><td>31.2</td></tr> <tr> <td>Isothermal expts. in a sealed glass tube</td><td>37.8; ADN: [NH<sub>4</sub><sup>+</sup>] 39.9; [N(NO<sub>2</sub>)<sub>2</sub>]<sup>-</sup> 35.3; gas products 36.3; 1% H<sub>2</sub>O, ADN [N(NO<sub>2</sub>)<sub>2</sub>]<sup>-</sup> 37.6; 20% H<sub>2</sub>O: ADN [N(NO<sub>2</sub>)<sub>2</sub>]<sup>-</sup></td></tr> <tr> <td>TGA (<math>u</math> = carrier gas flow rate, mL/min), <math>a</math> = extent of reaction</td><td>42 <math>u/a = 30/0.1</math> 40 <math>u/a = 100/0.1</math> 31 <math>u/a = 30/0.5</math> 36 <math>u/a = 100/0.5</math></td></tr> <tr> <td>DSC (thermal ignition in Wood's metal bath for 165–200 °C)</td><td>37.8 30.4</td></tr> </tbody> </table>	Exptl. conditions	$E_a$ (kcal/mol)	DSC (N <sub>2</sub> )	41.9	DSC (He)	43.1	DSC (sealed pan)	30.8	DSC ( $p = 37.42$ atm, air)	29.3	DSC ( $p = 37.42$ atm, He)	29.5	DSC (vacuum, 35 mm Hg)	31.2	Isothermal expts. in a sealed glass tube	37.8; ADN: [NH <sub>4</sub> <sup>+</sup> ] 39.9; [N(NO <sub>2</sub> ) <sub>2</sub> ] <sup>-</sup> 35.3; gas products 36.3; 1% H <sub>2</sub> O, ADN [N(NO <sub>2</sub> ) <sub>2</sub> ] <sup>-</sup> 37.6; 20% H <sub>2</sub> O: ADN [N(NO <sub>2</sub> ) <sub>2</sub> ] <sup>-</sup>	TGA ( $u$ = carrier gas flow rate, mL/min), $a$ = extent of reaction	42 $u/a = 30/0.1$ 40 $u/a = 100/0.1$ 31 $u/a = 30/0.5$ 36 $u/a = 100/0.5$	DSC (thermal ignition in Wood's metal bath for 165–200 °C)	37.8 30.4
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	<table border="1"> <thead> <tr> <th>Sample type</th><th>Enthalpy of dec. (kJ/g)</th></tr> </thead> <tbody> <tr> <td>Pristine ADN</td><td>1.86</td></tr> <tr> <td>Prilled, PS, 5 wt.%</td><td>3.35</td></tr> <tr> <td>Prilled HTPB, 5 wt.%</td><td>2.19</td></tr> <tr> <td>Sonicated, PS, 5 wt.%</td><td>1.81</td></tr> <tr> <td>Sonicated, HTPB, 5 wt.%</td><td>1.78</td></tr> <tr> <td>Sonicated, HTPB, 20 wt.%</td><td>2.62</td></tr> <tr> <td>Pristine ADN</td><td>1.97</td></tr> <tr> <td>Prilled ADN</td><td>2.01</td></tr> </tbody> </table>	Sample type	Enthalpy of dec. (kJ/g)	Pristine ADN	1.86	Prilled, PS, 5 wt.%	3.35	Prilled HTPB, 5 wt.%	2.19	Sonicated, PS, 5 wt.%	1.81	Sonicated, HTPB, 5 wt.%	1.78	Sonicated, HTPB, 20 wt.%	2.62	Pristine ADN	1.97	Prilled ADN	2.01		
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Enthalpy of dissolution [kcal/mol]	8.71 ± 0.01 <sup>[53]</sup>																				
Shrinkage on solidification	14.0% (NEXPLO sample) <sup>[55]</sup>																				
$K_{ow}$	0.05 l/kg <sup>[57]</sup>																				
$K_{oc}$	10.53 l/kg <sup>[57]</sup>																				
Bullet impact test [m/s]	309–316 (recryst. ADN, powder) <sup>[11]</sup>																				

	<b>ADN<sup>[14,41]</sup></b>	<b>ADN<sup>[15][16]</sup></b>	<b>ADN<sup>[4]</sup></b>	<b>ADN<sup>[4]</sup></b>	<b>ADN<sup>[4]</sup></b>	<b>ADN<sup>[11]</sup></b>
( $\alpha$ -ADN)	( $\beta$ -ADN)					Synchrotron radiation
Chemical formula	$\text{H}_4\text{N}_4\text{O}_4$	$\text{H}_4\text{N}_4\text{O}_4$	$\text{H}_4\text{N}_4\text{O}_4$	$\text{H}_4\text{N}_4\text{O}_4$	$\text{H}_4\text{N}_4\text{O}_4$	
Molecular weight [g mol <sup>-1</sup> ]	124.07	124.07	124.07	124.07	124.07	124.07
Crystal system	Monoclinic					Monoclinic
Space group	$P2_1/c$ (no. 14)					
$a$ [\AA]	6.914(1)	Unit cell parameters not reported	6.84	5.6228	6.933(1)	6.908
$b$ [\AA]	11.787(3)		11.90	11.8750	11.603(1)	11.895
$c$ [\AA]	5.614(1)		5.61	6.8954	5.567(1)	5.638
$\alpha$ [°]	90		90	90	90	90
$\beta$ [°]	100.40(1)		99.8	100.17	100.58	100.17(2)
$\gamma$ [°]	90		90	90	90	90
$V$ [\AA <sup>3</sup> ]	450.0(2)					453.19(11)
$Z$	4					
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.831		1.831	1.8184	1.872	1.807
$T$ [K]	223			293	90	295
						293

There are two crystalline ADN polymorphs:  $\alpha$ -ADN (low-pressure phase, stable  $\leq 20$  GPa @  $-71 \leq T \leq 120$  °C) and  $\beta$ -ADN (stable  $> 2.0$  GPa @  $-75$  °C  $\geq T \geq 140$  °C)<sup>[15,16]</sup>; both  $\alpha$ -ADN and  $\beta$ -ADN undergo irreversible thermal dec. @ mpt.<sup>[15]</sup> At 1–10 GPa @  $T > 140$  °C, dec. of ADN  $\rightarrow$  AN + N<sub>2</sub>O<sup>[16]</sup>

Crystal types obtained from various solvents<sup>[22]</sup>:

Propylene carbonate, needle shaped<sup>[22]</sup>; 1-propanol, needle shaped<sup>[22]</sup>; 1-pentanol, needle shaped<sup>[22]</sup>; 1-octanol, needle shaped<sup>[22]</sup>; benzyl alcohol, short, compact needles<sup>[22]</sup>; 2-methyl-2-pentanol, needle shaped<sup>[22]</sup>; ethylene glycol, needle shaped<sup>[22]</sup>; *n*-butyl acetate, short needles<sup>[22]</sup>;  $\gamma$ -butyrolactone, long needles<sup>[22]</sup>; diethylene glycol monoethyl ether, needle shaped<sup>[22]</sup>

X-ray: relative linear expansion coefficients of ADN lattice<sup>[30]</sup>:

Lattice parameter	$T < 0$ °C	$0$ °C $< T < 55$ °C	$55$ °C $< T < 65$ °C
$a$ ( $10^{-6}$ /°C)	-11	6	120
$b$ ( $10^{-6}$ /°C)	119	148	251
$c$ ( $10^{-6}$ /°C)	64	80	167
Vol. ( $10^{-6}$ /°C)	176	240	544

Relative change in cell parameters versus temperature (Fig. 1)<sup>[11]</sup>:

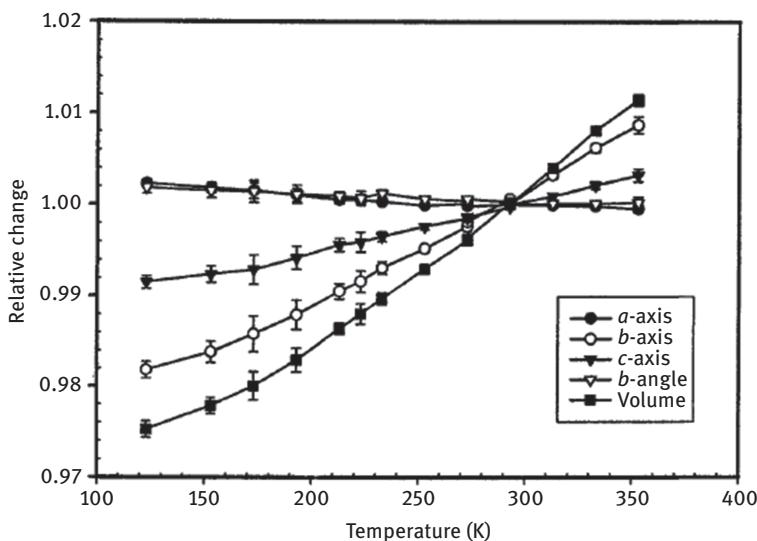


Fig. 1: Relative change of cell dimensions versus temperature<sup>[11]</sup>.

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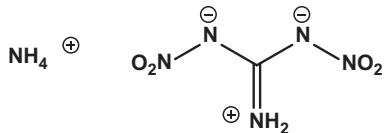
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## Ammonium dinitroguanidine

Name [German, acronym]: Dinitroguanidine, ammonium salt [ammonium dinitroguanidin, ADNQ]

Main (potential) use: gas generant

Structural formula:



	<b>ADNQ</b>		
Formula	$\text{CH}_6\text{N}_6\text{O}_4$		
Molecular mass [g mol <sup>-1</sup> ]	166.09		
Appearance at RT	Colorless crystals <sup>[1]</sup>		
IS [J]	10 (100–500 µm, BAM) <sup>[1]</sup>		
FS [N]	252 (100–500 µm, BAM) <sup>[1]</sup>		
ESD [J]	0.4 (100–500 µm, OZM apparatus) <sup>[1]</sup>		
N [%]	50.60		
$\Omega(\text{CO}_2)$ [%]	-9.63		
$T_{\text{dec.}}$ [°C]	197 (exo, onset, DSC @ 5 °C/min, covered Al pans with hole in lid) <sup>[1]</sup>		
$\rho$ [g cm <sup>-3</sup> ]	1.735 (X-ray @ 173 K) <sup>[1]</sup>		
Heat of formation	-6.4 kJ/mol ( $\Delta_f H^\circ$ , (s), calcd., CBS-4M) <sup>[1]</sup> , 81 kJ/kg ( $\Delta_f U^\circ$ , (s), calcd., CBS-4M) <sup>[1]</sup>		
	Calcd. (EXPLO5 5.03)	Lit. values	Exptl.
$-\Delta_{\text{ex}} U^\circ$ [kJ kg <sup>-1</sup> ]	5,193 <sup>[1]</sup>		
$T_{\text{ex}}$ [K]	3,828 <sup>[1]</sup>		
$p_{\text{CJ}}$ [kbar]	327 <sup>[1]</sup>		

VoD [ $\text{m s}^{-1}$ ]	9,066 (@ 1.735 g $\text{cm}^{-3}$ ) <sup>[1]</sup>		
$V_0$ [L $\text{kg}^{-1}$ ]	934		
Thermal stability	No dec. or mass loss in Radex oven @ 75 °C for 48 h <sup>[1]</sup>		

	<b>ADNQ<sup>[1]</sup></b>
Chemical formula	$\text{CH}_6\text{N}_6\text{O}_4$
Molecular weight [g $\text{mol}^{-1}$ ]	166.09
Crystal system	Monoclinic
Space group	$P2_1/c$ (no. 14)
$a$ [\mathring{A}]	10.7925
$b$ [\mathring{A}]	6.2994
$c$ [\mathring{A}]	10.6651
$\alpha$ [°]	90
$\beta$ [°]	118.679
$\gamma$ [°]	90
$V$ [\mathring{A} <sup>3</sup> ]	636.13(8)
$Z$	4
$\rho_{\text{calc}}$ [g $\text{cm}^{-3}$ ]	1.735
$T$ [K]	173
	Recryst. from EtOH/water mixture

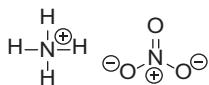
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## Ammonium nitrate

Name [German, acronym]: Ammonium nitrate [ammoniumnitrat, ammonalsalpeter, Sprengsalpeter, AN]

Main (potential) use: Oxidizer, component of binary explosives<sup>[3]</sup>, component of dynamites, cratering explosives and some rocket propellants<sup>[3]</sup>, oxidizer in solid propellants, explosives and gas-generating systems<sup>[36]</sup>, uses limited by its hygroscopicity<sup>[38]</sup>, base component of some recent gas generators<sup>[47]</sup>, possible substitute for AP<sup>[47]</sup>, component of pyrotechnic composite mixtures<sup>[47]</sup>, principal component of most industrial explosives<sup>[54]</sup>, gas generator for turbo pumps of liquid propellant engines<sup>[54]</sup>, emergency starters for jet aircraft<sup>[54]</sup>, used alone as cratering charge and in ditching and quarrying<sup>[56]</sup>, used in mixtures for bombs or large caliber shells<sup>[56]</sup>, in combination with TNT used for filling shells<sup>[60]</sup>, component of ammonia dynamites<sup>[60]</sup>, principal component of some common blasting agents<sup>[71]</sup>, occasionally used in rocket propellants<sup>[71]</sup>

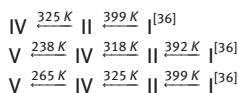
Structural formula:



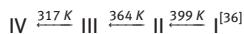
	<b>Ammonium nitrate</b>
Formula	$\text{NH}_4\text{NO}_3$
Molecular mass [g mol <sup>-1</sup> ]	80.04
Appearance at RT	Colorless crystals, white solid <sup>[32,54,59,71]</sup> , crystalline white solid <sup>[47,60]</sup> , white powder <sup>[56]</sup> , colorless salt <sup>[67]</sup> , odorless, transparent deliquescent crystals or white granules <sup>[73]</sup>
IS [J]	>40 (<100 µm), >50 <sup>[6]</sup> , 100+ cm (19.62 J, 2 kg mass, B.M.) <sup>[3,4]</sup> , 31 in (2 kg mass, 15.45 J, P.A.) <sup>[3,4]</sup> , 19.6 (>100 cm, 2 kg mass, 20 mg sample, B.M.) <sup>[7]</sup> , 15.5 (31 in, 17 mg sample, P.A.) <sup>[7]</sup> , >49 <sup>[10]</sup> , 31 in (2 kg mass, P.A.) <sup>[17]</sup> , $H_{50\%} > 320$ cm (US NOL) <sup>[18]</sup> , $H_{50\%} 320$ cm (2.5 kg hammer, 35 mg sample, US NOL) <sup>[41]</sup> , $H_{50\%} \geq 320$ cm (2.5 kg mass, type 12 tool, ERL method) <sup>[63]</sup> , limiting impact energy $\geq 50$ J (BAM) <sup>[74]</sup> , $H_{50} = 2$ go's @ 320 cm (type 12) <sup>[76]</sup> , $H_{50} \geq 320$ cm (type 12B) <sup>[76]</sup> , $H_{50}$ (average) $\geq 337$ cm (design no. 7 apparatus, 5 kg mass) <sup>[78]</sup> , $H_{50} = 328$ cm (design no. 12 apparatus, 394 units, cf. TNT = 100 units) <sup>[78]</sup>

	P.A. values (2 kg mass): 15.45 (31 in @ 25 °C) <sup>[7,26]</sup> , 13.96 (28 in @ 75 °C) <sup>[7,26]</sup> , 13.46 (28 in @ 100 °C) <sup>[7,26]</sup> , 13.46 (27 in @ 150 °C) <sup>[7,26]</sup> , 5.98 (12 in @ 175 °C) <sup>[7,26]</sup>																		
FS [N]	>360 (<100 µm), >363 <sup>[6]</sup> , 353 <sup>[10]</sup> , cannot be detonated by steel shoe <sup>[7,59]</sup> , unaffected by fiber shoe (friction pendulum test) <sup>[7]</sup> , unaffected by steel shoe (friction pendulum test) <sup>[26]</sup> , limiting load ≥363 N <sup>[74]</sup>																		
ESD [J]	>1.5 (<100 µm), $E_{50\%} = 0.58 \pm 0.10$ (Bruceton) <sup>[42]</sup>																		
N [%]	34.98																		
Ω [%]	+19.99																		
$T_{\text{phase transitions}}$ [°C]	-18 (tetragonal → orthorhombic) <sup>[14]</sup> , 32.1 (orthorhombic → orthorhombic) <sup>[14]</sup> , 84.2 (orthorhombic → tetragonal) <sup>[14]</sup> , 125.2 (tetragonal → cubic) <sup>[14]</sup> , 169.6 (cubic → liquid) <sup>[14]</sup> , -18 (tetragonal → orthorhombic) <sup>[16]</sup> , 32.1 (orthorhombic → orthorhombic) <sup>[16]</sup> , 84.2 (orthorhombic → tetragonal) <sup>[16]</sup> , 125.2 (tetragonal → cubic) <sup>[16]</sup> , 169.9 (cubic → liquid) <sup>[16]</sup> , 32.2 (AN IV → AN III) <sup>[8]</sup> , 2–5 [AN-V → AN-IV (small grains)] <sup>[15]</sup>																		
Thermal stability of phases <sup>[15]</sup> :																			
<table border="1"> <thead> <tr> <th>Phase</th> <th>Crystal system</th> <th>Stability (°C)</th> </tr> </thead> <tbody> <tr> <td>AN-V</td> <td>Orthorhombic</td> <td>&lt; -18</td> </tr> <tr> <td>AN-IV</td> <td>Orthorhombic</td> <td>-18 to 55</td> </tr> <tr> <td>AN-III</td> <td>Orthorhombic</td> <td>32–84 (wet) Nonexistent (dry)</td> </tr> <tr> <td>AN-II</td> <td>Tetragonal</td> <td>55–125 (dry)</td> </tr> <tr> <td>AN-I</td> <td>Cubic</td> <td>&gt;125 (dry)</td> </tr> </tbody> </table>		Phase	Crystal system	Stability (°C)	AN-V	Orthorhombic	< -18	AN-IV	Orthorhombic	-18 to 55	AN-III	Orthorhombic	32–84 (wet) Nonexistent (dry)	AN-II	Tetragonal	55–125 (dry)	AN-I	Cubic	>125 (dry)
Phase	Crystal system	Stability (°C)																	
AN-V	Orthorhombic	< -18																	
AN-IV	Orthorhombic	-18 to 55																	
AN-III	Orthorhombic	32–84 (wet) Nonexistent (dry)																	
AN-II	Tetragonal	55–125 (dry)																	
AN-I	Cubic	>125 (dry)																	
DTA (@ 15 °C/min, crystalline transitions): 35–50 (endo), 33 (DTA transition $\mathcal{T}$ ) (rhombic-II → rhombic-I); 76–101 (endo) 89 (DTA transition $\mathcal{T}$ ) (rhombic-I → tetragonal); 117–141 (endo) 129 (DTA transition $\mathcal{T}$ ) (tetragonal → cubic) <sup>[23]</sup>																			
Transition paths of AN <sup>[36]</sup> :																			
Transition paths of AN <sup>[51]</sup> :																			
(* AN humid)																			

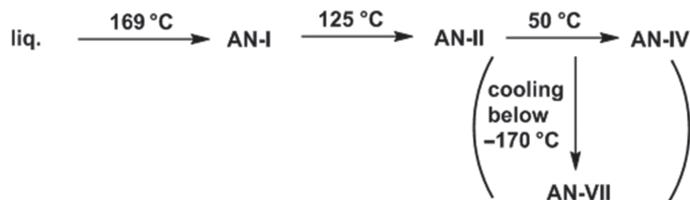
Dry AN cycled from RT to 425 K; on cooling, transitions into phases II, IV and V observed, and during the second heating the transitions occurred in the reverse order<sup>[36]</sup>:



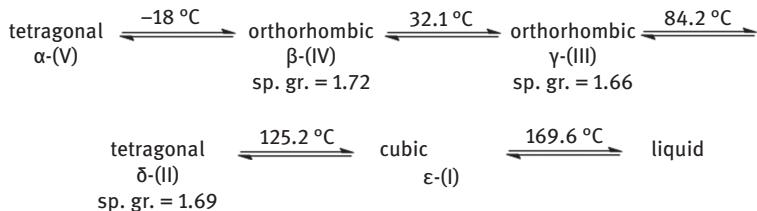
When samples were cooled to 173 K before starting the measurements @ 203 K, mixtures of phases IV and V were observed<sup>[36]</sup>:



*Volfkovich*<sup>[38]</sup>: only three transformations observed when molten AN is cooled @ 2 °C/min (i.e., quickly cooled)<sup>[38]</sup>:



AN occurs in five crystalline modifications<sup>[38]</sup>:



@  $T > 169\text{ °C}$  and  $p > 9,000\text{ kg/cm}^2$  Bridgman has established the existence of one more form (VI)<sup>[38]</sup>, 53 (endo, solid phase IV  $\rightarrow$  solid phase II), 125 (endo, solid phase II  $\rightarrow$  solid phase I) (DSC @ 10 K/min, 2.2 mg sample, dry  $\text{N}_2$  atmosphere, PSAN (phase-stabilized AN) – i.e., AN with Ni, Cu or Zn oxides which promote phase IV changing directly to phase II which avoids the large vol. expansion that occurs when phase IV changes to phase III @ 32 °C)<sup>[47]</sup>

*Théorêt*: AN is known in seven crystalline modifications<sup>[49]</sup>; phase I (cubic, @ 169–125 °C), phase II (tetragonal, @ 125–84.5 °C), phase III (orthorhombic, @ 84.5–32 °C), phase IV (orthorhombic, @ 32 to –16 °C), phase V (tetragonal, less than –16 °C), phase VI (>169 °C @ pressures >9,000 kg/cm<sup>2</sup>), phase VII (less than –170 °C)<sup>[49]</sup>

*Quaresma* (DSC @ 5 °C/min, open alumina cup): AN observed in five of the seven phases described by Théorêt; phase IV (orthorhombic, RT to 40.5 °C, phase transition to phase III then occurs), phases IV (orthorhombic) and III (orthorhombic) both present @ 40.5–55.6, phase IV → phase II @ 55.6 °C, phases III (orthorhombic) and II (tetragonal) present @ 55.6–92.6 °C, phase III → phase II @ 92.6 °C, phase II (tetragonal) @ 92.6–129.6 °C, phase II → phase I @ 129.6 °C<sup>[49]</sup> ~ –178 (phase transition V → VII)<sup>[54]</sup>, –27 (phase transition IV → V)<sup>[54]</sup>, phase I = highest temperature phase<sup>[54]</sup>, 32 (phase IV → phase III)<sup>[54]</sup>, phase I: cubic, 170–125 °C<sup>[54]</sup>, phase II: tetragonal, 125–84 °C<sup>[54]</sup>, phase III: orthorhombic, 84–32 °C<sup>[54]</sup>, phase IV: orthorhombic, 32 to –16 °C<sup>[54]</sup>, phase V: tetragonal, less than –16 °C<sup>[54]</sup>, phase I remains stable up to mpt.<sup>[54]</sup>

Values from<sup>[26]</sup>:

Form	Crystal system	Range (°C)
Liquid		> 169.6
I epsilon	Regular (cubic) (isometric)	125.0 to 169.6
II delta	Rhombohedral or tetragonal	84.1 to 125
III gamma	Orthorhombic	32.3 to 84.1
IV beta	Orthorhombic	–18 to 32.2
V alpha	Tetragonal	–18 to –150

AN exists in five crystalline forms which are stable as follows<sup>[67]</sup>:

Form	Stable range (°C)
α (or V)	Less than –16
β (or IV)	–16 → +32
γ (or III)	32 → 84
δ (or II)	84 → 125
ξ (or I)	125 → mpt.

Five solid phases exist @ normal pressure: orthorhombic @ RT<sup>[73]</sup>

$T_{m.p.}$ [°C]	169.5 <sup>[3]</sup> , 170 <sup>[7,21,65,71]</sup> , 169 <sup>[8,10,14,24]</sup> , 169.6–169.9 (with slight sublimation) <sup>[17]</sup> , ~165 (technical grade) <sup>[17]</sup> , 50 (endo), 84 (endo), 126 (endo) 160 (endo), 285 (exo) (DTA, Pt cups, @ atmospheric pressure) <sup>[37]</sup> , 52 (endo), 126 (endo), 172 (endo), 209 (endo) (exo–endo change in final peak, predominantly dissociation process leading to evaporation/sublimation which is endo) (DTA, Pt cups, @ 0.5 mm Hg pressure) <sup>[37]</sup> , 169.6 (crystals) <sup>[38,59]</sup> , 169 (endo, DSC @ 10 K/min, 2.2 mg sample, dry N <sub>2</sub> atmosphere, PSAN – i.e., AN with Ni, Cu or Zn oxides which promote phase IV changing directly to phase II which avoids the large vol. expansion that occurs when phase IV changes to phase III @ 32 °C) <sup>[47]</sup> , 170.9 (DSC @ 5 °C/min, open alumina cup) <sup>[49]</sup> , 169–171 <sup>[51]</sup> , 169.9 <sup>[53]</sup> , 169.6 <sup>[54,75]</sup> , 167 (heat flux curve, @ 0.2 °C/min, 2.0 g sample) <sup>[54]</sup> , 163–170 <sup>[56]</sup> , 155–166 <sup>[60]</sup> , 170 (if pure and dry) <sup>[67]</sup>
$T_{b.p.}$ [°C]	210 <sup>[26,49]</sup> , 210 @ 11 mm Hg (and distills without dec.) <sup>[54,59]</sup>

$T_{dec}$ [°C]	210 <sup>[7,10,60]</sup> , 210 <sup>[8,34,52]</sup> , >230 (@ 760 mm Hg) <sup>[17]</sup> , ~250 (onset, DTA @ 5 °C/min) <sup>[5]</sup> , 284 (onset, DSC @ 5 K/min) <sup>[6]</sup> , 273 (TG inflection point, mass loss = 17%) <sup>[22]</sup> , 50 (endo), 84 (endo), 126 (endo), 169 (endo), 285 (exo) (DTA peak max. @ atmospheric pressure) <sup>[22]</sup> , 52 (endo), 126 (endo), 172 (endo), 209 (endo) (DTA peak max. @ 0.5 mm Hg pressure) <sup>[22]</sup> , 170 (fusion), 249 (rapid bubbling), 289 (vigorous bubbling), 395 (rapid nitrous fumes) <sup>[23]</sup> , 230 <sup>[26]</sup> , 328 (exo peak max., DSC @ 20 °C/min) <sup>[24]</sup> , 285 (exo) (DTA, Pt cups, @ atmospheric pressure) <sup>[37]</sup> , 273 (DTA inflection point, 97% weight loss) <sup>[37]</sup> , 210 (exo, DSC @ 10 K/min, 2.2 mg sample, dry N <sub>2</sub> atmosphere, PSAN – i.e., AN with Ni, Cu or Zn oxides which promote phase IV changing directly to phase II which avoids the large vol. expansion that occurs when phase IV changes to phase III @ 32 °C) <sup>[47]</sup> , ~220 (start of dec., TGA, 5–10 mg sample, 10 °C/min, covered Al pans) <sup>[48]</sup> , 250 extending to 282.1 (DSC @ 5 °C/min, open alumina cup) <sup>[49]</sup> , ~230 (@ 760 mm Hg (deflagrates >325 °C) <sup>[54]</sup> , 300 (exo, onset), 327 (exo, peak max) (DSC @ 20 °C/min) <sup>[55]</sup> , dec. > mpt. at atmospheric pressure <sup>[59]</sup> , 220 (dec. begins) <sup>[67]</sup> , ~210 (orthorhombic) <sup>[73]</sup> , 284 (DSC) <sup>[74]</sup>			
TG-DSC ( $T_0$ = onset $T$ of dec., $T_p$ = peak $T$ , $T_e$ = end $T$ of dec., $\beta$ = heating rate) <sup>[64]</sup> :				
$\beta$ (°C/min)	$\Delta H$ (J/g)	$T_0$ (°C)	$T_p$ (°C)	$T_e$ (°C)
2.5	-1,613	178.6	258.4	268.4
5	-1,355	185.0	278.3	301.1
10	-1,107	196.8	294.8	326.4
15	-1,049	201.3	303.4	349.1
$\rho$ [g cm <sup>-3</sup> ]	1.722 (@ 298 K, crystal), 1.73 (crystal) <sup>[7,65]</sup> , 1.725 <sup>[8,32,47,49,52,54]</sup> , 1.724 (@ 298 K) <sup>[1]</sup> , 1.725 (cryst. @ 25 °C) <sup>[17]</sup> , 1.402 (molten AN @ 175 °C) <sup>[17]</sup> , 1.36 (molten AN @ 200 °C) <sup>[17]</sup> , 1.594 (AN-I ( $\epsilon$ -) @ 130 °C) (range = 125.2–169.6 °C) <sup>[17]</sup> , 1.667 (AN-II ( $\delta$ -)) @ 93 °C (range = 84.2–125.2 °C) <sup>[17]</sup> , 1.661 (AN-III ( $\gamma$ -) @ 40 °C) (range = 32.1–84.2 °C) <sup>[17]</sup> , 1.725 (AN-IV ( $\beta$ -) @ 25 °C) (range = -16–32.1 °C) <sup>[17]</sup> , 1.710 (AN-V ( $\alpha$ -) @ -25 °C) (range = -18 to -16 °C) <sup>[17]</sup> , 1.725 <sup>[34]</sup> , 1.58–1.61 (AN-I ( $\epsilon$ -) stable in $T$ range 125–169.6) <sup>[26]</sup> , 1.64–1.67 (AN-II ( $\delta$ -) stable in $T$ range 84.1–125.0) <sup>[26]</sup> , 1.64–1.66 (AN-III ( $\gamma$ -) stable in $T$ range 32.8–84.1) <sup>[26]</sup> , 1.71–1.75 (AN-IV ( $\beta$ -) stable in $T$ range -18 to 32.3) <sup>[26]</sup> , 1.70–1.72 (AN-V ( $\alpha$ -) stable in $T$ range -18 to -150) <sup>[26]</sup> , 1.402 (molten AN @ 175 °C) <sup>[26]</sup> , 1.36 (molten AN @ 200 °C) <sup>[26]</sup> , sp. gr. = 1.725 <sup>[60]</sup> , 1.72 <sup>[51,71]</sup> , 1.72 (orthorhombic) <sup>[73]</sup>			
Heat of formation	-366 kJ/mol (enthalpy of form.) <sup>[71]</sup> , -87.37 kcal/mol ( $\Delta H_f^\circ$ ) <sup>[45]</sup> , -351 kJ/mol ( $H_f$ ) <sup>[47]</sup> , -365.1 kJ/mol ( $\Delta H_f$ ) <sup>[8]</sup> , -87.4 kcal/mol <sup>[9]</sup> , -396 kJ mol <sup>-1</sup> <sup>[10]</sup> , -1,090 cal/g <sup>[1]</sup> , -88.6 kcal mol <sup>-1</sup> <sup>[17,26,38]</sup> , -351 kJ mol <sup>-1</sup> ( $H_f$ ) <sup>[32]</sup> , -97.37 kcal mol <sup>-1</sup> ( $\Delta H_f^\circ$ exptl.) <sup>[33]</sup> , -87.08 kcal/mol ( $\Delta H_f^\circ$ calcd.) <sup>[33]</sup> , -344.26 kJ/mol (enthalpy of form.) <sup>[34,49,52]</sup> , -365.6 kJ/mol ( $\Delta H_f^\circ$ ) <sup>[53]</sup> , -4,567.5 J/g ( $\Delta H_f^\circ$ ) <sup>[53]</sup> , 4,594 J/g <sup>[54]</sup> , 87 kcal/mol (@ constant pressure) <sup>[59]</sup> , -365.7 kJ/mol ( $\Delta H_f^\circ$ , exptl.) <sup>[77]</sup> , -341.0 kJ/mol ( $\Delta H_f^\circ$ , calcd., Born–Haber cycles) <sup>[77]</sup>			

Heat of combustion	346 cal/g <sup>[7,65]</sup> , 627.8 cal/g ( $Q_c^V$ ) <sup>[17]</sup> , 50.3 kcal mol <sup>-1</sup> ( $Q_c^V$ ) <sup>[17,26]</sup> , 616.9 cal/g ( $Q_c^P$ ) <sup>[17]</sup> , 49.4 kcal/mol ( $Q_c^P$ ) <sup>[17,26]</sup> , 346 kcal/kg <sup>[18]</sup> , 210.47 kJ/mol <sup>[34]</sup> , heat of combustion/enthalpy of reaction = 210.47 kJ/mol <sup>[49,52]</sup> , 1,447.7 J/g <sup>[54]</sup> , 628 cal/g <sup>[59]</sup> , $\Delta H_c = -78$ kcal/mol <sup>[61]</sup>		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{ex}U^\circ$ [kJ kg <sup>-1</sup> ]	1,577	1,712 (calcd., ZMW Cyw) <sup>[5]</sup> 2,479 [H <sub>2</sub> O (l) @ 25 °C] (calcd., ICT thermodynamic code) <sup>[13]</sup> 335 cal/g <sup>[25]</sup> 630 cal/g ( $Q_e^V$ , calcd., [H <sub>2</sub> O (l)]) <sup>[17]</sup> 346.3 cal/g ( $Q_e^V$ , calcd., [H <sub>2</sub> O (g)] using different rxn.) <sup>[17]</sup> 375 cal/g [H <sub>2</sub> O (l)] <sup>[17]</sup> 347 (cal/g @ 1.0 g cm <sup>-3</sup> ) <sup>[17]</sup> 346 kcal/kg <sup>[18]</sup> 1,470 (850 kg/m <sup>3</sup> , calcd., TIGER, JCZ3) <sup>[35]</sup> 1,480 (850 kg/m <sup>3</sup> , calcd., TIGER, BKW) <sup>[35]</sup> 1,480 (850 kg/m <sup>3</sup> , calcd., KHT) <sup>[35]</sup> 1,620 (850 kg/m <sup>3</sup> , calcd., DTONATE, Cook) <sup>[35]</sup> 2,479 J/g [H <sub>2</sub> O (g)] (calcd., ICT thermodynamic code) <sup>[53]</sup> 346 cal/g <sup>[59]</sup> 1,440 [H <sub>2</sub> O (g)] <sup>[71]</sup>	346 cal/g (heat of explosion) <sup>[7,65]</sup> 1,448 <sup>[7]</sup> 630 cal/g <sup>[39]</sup>

$T_{\text{ex}}$ [K]	1,576	1,500 °C (est.) <sup>[17]</sup> 2,120 (calcd.) <sup>[17]</sup>  1,660 (850 kg/m <sup>3</sup> , calcd., TIGER, JCZ3) <sup>[35]</sup>  1,080 (850 kg/m <sup>3</sup> , calcd., TIGER, BKW) <sup>[35]</sup>  1,290 (850 kg/m <sup>3</sup> , calcd., KHT) <sup>[35]</sup>  1,820 (850 kg/m <sup>3</sup> , calcd., DTONATE, Cook) <sup>[35]</sup>  470 (@ 1.725 g cm <sup>-3</sup> , calcd., TIGER BKW) <sup>[68]</sup>  1,177 (@ 1.725 g cm <sup>-3</sup> , calcd., TIGER BKWR) <sup>[68]</sup>  1,120 (@ 1.725 g cm <sup>-3</sup> , calcd., LJD) <sup>[68]</sup>	1,125 °C (calcd. based on expts. measuring pressure in manometric bomb) <sup>[39]</sup>  2,120 °C <sup>[39]</sup>
$p_{\text{CJ}}$ [kbar]	216	65.8 GPa (@ 1.05 g cm <sup>-3</sup> , calcd. empirical, Xiong) <sup>[25]</sup>  3.5 GPa (850 kg/m <sup>3</sup> , calcd., TIGER, JCZ3) <sup>[35]</sup>  4.9 GPa (850 kg/m <sup>3</sup> , calcd., TIGER, BKW) <sup>[35]</sup>  3.9 GPa (850 kg/m <sup>3</sup> , calcd., KHT) <sup>[35]</sup>  2.7 GPa (850 kg/m <sup>3</sup> , calcd., DTONATE, Cook) <sup>[35]</sup>  182 (@ 1.725 g cm <sup>-3</sup> , calcd., KSM) <sup>[68]</sup>  210 (@ 1.725 g cm <sup>-3</sup> , calcd., TIGER BKW) <sup>[68]</sup>  190 (@ 1.725 g cm <sup>-3</sup> , calcd., TIGER BKWR) <sup>[68]</sup>  217 (@ 1.725 g cm <sup>-3</sup> , calcd., LJD) <sup>[68]</sup>	

VoD [ $\text{m s}^{-1}$ ]	7,960	<p>2,800 (@ 1.0 <math>\text{g cm}^{-3}</math>)<sup>[19]</sup></p> <p>4,639 (@ 1.05 <math>\text{g cm}^{-3}</math>, calcd., empirical, <i>Xiong</i>)<sup>[25]</sup></p> <p>4,010 (850 <math>\text{kg/m}^3</math>, calcd., TIGER, JCZ3)<sup>[35]</sup></p> <p>4,710 (850 <math>\text{kg/m}^3</math>, calcd., TIGER, BKW)<sup>[35]</sup></p> <p>4,230 (850 <math>\text{kg/m}^3</math>, calcd., KHT)<sup>[35]</sup></p> <p>3,600 (850 <math>\text{kg/m}^3</math>, calcd., DTONATE, <i>Cook</i>)<sup>[35]</sup></p> <p>2,360 (@ 0.5 <math>\text{g cm}^{-3}</math>, calcd., predicted max. speed)<sup>[57]</sup></p> <p>2,560 (@ 0.6 <math>\text{g cm}^{-3}</math>, calcd., predicted max. speed)<sup>[57]</sup></p> <p>2,760 (@ 0.7 <math>\text{g cm}^{-3}</math>, calcd., predicted max. speed)<sup>[57]</sup></p> <p>2,980 (@ 0.8 <math>\text{g cm}^{-3}</math>, calcd., predicted max. speed)<sup>[57]</sup></p> <p>3,220 (@ 0.9 <math>\text{g cm}^{-3}</math>, calcd., predicted max. speed)<sup>[57]</sup></p> <p>3,480 (@ 1.0 <math>\text{g cm}^{-3}</math>, calcd., predicted max. speed)<sup>[57]</sup></p> <p>3,460 (@ 1.00 <math>\text{g cm}^{-3}</math>, calcd., K-W eq.)<sup>[58]</sup></p> <p>6,000 (@ 1.725 <math>\text{g cm}^{-3}</math>, calcd., Taylor method)<sup>[68]</sup></p> <p>6,490 (@ 1.725 <math>\text{g cm}^{-3}</math>, calcd., KSM)<sup>[68]</sup></p> <p>7,840 (@ 1.725 <math>\text{g cm}^{-3}</math>, calcd., TIGER BKW)<sup>[68]</sup></p>	<p>4,500 (@ 1.05 <math>\text{g cm}^{-3}</math>)<sup>[2, 29]</sup></p> <p>1,000 (@ 0.9 <math>\text{g cm}^{-3}</math>, solid, no confinement, 1.25 in charge diameter)<sup>[3, 7]</sup></p> <p>2,500 (@ 1.4 <math>\text{g cm}^{-3}</math>, liquid, strong confinement, 4.5 in charge diameter)<sup>[3, 7]</sup></p> <p>1,650 (@ 0.826 <math>\text{g cm}^{-3}</math>)<sup>[5]</sup></p> <p>~1,500 (@ 0.7 <math>\text{g cm}^{-3}</math>)<sup>[8, 9]</sup></p> <p>2,700 (@ 1.73 <math>\text{g cm}^{-3}</math>)<sup>[12]</sup></p> <p>2,800 (@ 1.0 <math>\text{g cm}^{-3}</math>)<sup>[26]</sup></p> <p>2,700 (@ 0.98 <math>\text{g cm}^{-3}</math>, 30 mm diameter steel tube)<sup>[26]</sup></p> <p>1,400 (@ 0.52 <math>\text{g cm}^{-3}</math>, lightweight cellulose acetate or cardboard tube, 1.5 in diameter, initiated by primers of blasting gelatin)<sup>[57]</sup></p> <p>1,550 (@ 0.52 <math>\text{g cm}^{-3}</math>, lightweight cellulose acetate or cardboard tube, 2 in diameter, initiated by primers of blasting gelatin)<sup>[57]</sup></p> <p>1,780 (@ 0.52 <math>\text{g cm}^{-3}</math>, lightweight cellulose acetate or cardboard tube, 3 in diameter, initiated by primers of blasting gelatin)<sup>[57]</sup></p> <p>1,950 (@ 0.52 <math>\text{g cm}^{-3}</math>, lightweight cellulose acetate or cardboard tube, 3 in diameter, initiated by primers of blasting gelatin)<sup>[57]</sup></p>
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		<p>7,430 (@ 1.725 g cm<sup>-3</sup>, calcd., TIGER BKWR)<sup>[68]</sup></p> <p>7,680 (@ 1.725 g cm<sup>-3</sup>, calcd., LJD)<sup>[68]</sup></p> <p>2,700 (@ 1.72 g cm<sup>-3</sup>)<sup>[71]</sup></p>	<p>2,050 (@ 0.52 g cm<sup>-3</sup>, lightweight cellulose acetate or cardboard tube, 5.5 in diameter, initiated by primers of blasting gelatin)<sup>[57]</sup></p> <p>2,230 (@ 0.52 g cm<sup>-3</sup>, lightweight cellulose acetate or cardboard tube, 7<sup>3</sup>/4 in diameter, initiated by primers of blasting gelatin)<sup>[57]</sup></p> <p>(see later tables)</p>
$V_0$ [L kg <sup>-1</sup> ]	1,069	<p>992 dm<sup>3</sup>/kg (calcd., ZMWCyw)<sup>[5]</sup></p> <p>980 (calcd., ZMWCyw)<sup>[11]</sup></p> <p>459 (calcd., ICT thermodynamic code)<sup>[13]</sup></p> <p>459 cm<sup>3</sup>/g (thermodynamically controlled combustion @ 25 °C without water, ICT thermodynamic code)<sup>[53]</sup></p> <p>980<sup>[59]</sup></p>	<p>980<sup>[7,65]</sup></p> <p>945 (incomplete detonation)<sup>[17]</sup></p> <p>980 (complete detonation)<sup>[26]</sup></p> <p>937 L (specific vol. is vol. @ 0 °C and 760 mm Hg for (g) products of explosion)<sup>[39]</sup></p>

All values determined experimentally<sup>[17]</sup>:

Rates of detonation (m/s)	$\rho$ (g cm <sup>-3</sup> )	Charge diameter (mm)	Initiation by no. 8 cap and container type	Charge $T$ (if not RT) (°C)
1,140	0.68–0.73	26.2	75 g tetryl, Shelby tube	15
1,560	0.68–0.73	26.2	75 g tetryl, 53.5 cm long, 4.85 mm wall	71
1,230	0.69	50	100 g PA, steel tube	
1,310	0.84	25	50 g tetryl, steel tube	
1,470	0.83	26	60 g tetryl, steel tube	
1,530	0.79	80	100 g PA, steel tube	
1,550	0.88	80	100 g PA, steel tube	
1,820	0.84	100	200 g PA, steel tube	

1,850	0.82	26.2	100 g tetryl, Shelby tube	
1,920	0.64	100	100 g PA, steel tube	
2,440	—	50	100 g PA, lead tube	
2,700	0.98	80	250 g tetryl, steel tube	

Detonation rates in steel tubes of different sizes<sup>[17]</sup>:

Size of steel tube (in)	$\rho$ (g cm <sup>-3</sup> )	Detonation rate (m/s)
5	0.96	2,570
4	0.96	1,681
3	0.96	Failure

Experimentally determined VoD values, AN confined in steel tubes, AN initiated by booster over the whole cross section of the tube. Booster=50 mm thickness, plastic explosive (PETN/oil, 88/12,  $\rho=1,550$  kg/m<sup>3</sup>), VoD measured using continuous velocity probe, low-density prilled AN<sup>[35]</sup>:

Inner diameter (mm)	Outer diameter (mm)	Wall thickness (mm)	Tube length (mm)	Loading $\rho$ (kg/m <sup>3</sup> )	VoD (km/s)
104	114	5	1,000	820	Decay
				830	1.80
				850	1.70
				850	Decay
98	114	8	1,000	830	2.20 <sup>†</sup>
				830	2.20 <sup>†</sup>
100	120	10	1,000	830	2.50
				840	2.60
				830	2.65
101	133	16	1,000	820	2.70
				820	2.80
100	140	20	1,000	820	2.90
				820	3.05
				820	3.10 <sup>†</sup>
				820	3.20

102	161	29	1,000	820	2.95
				820	3.00
49	69	10	1,160	850	Decay
100	120	10	1,000	830	2.50
				840	2.60
				830	2.65
148	168	10	1,000	820	2.85
				820	3.20
199	219	10	1,000	820	3.40
				820	3.50
				830	3.60 <sup>‡</sup>
				830	3.60 <sup>‡</sup>
254	274	10	600	820	3.75
				840	3.80
303	323	10	600	830	3.95
192	200	4 (PVC)	1,000	830	Decay
				840	Decay
207	247	20	1,000	830	3.60
52	102	25	1,000	820	Decay
				840	Decay

<sup>†</sup>Performed under earth cover; <sup>‡</sup>performed in open air.

Critical diameter [cm]	Steady propagation observed down to 2 in diameter over at least a 2 ft length of charge and at 1.5 in at diameter over a 9 in length, at 1 in diameter the wave died out quickly ( $\rho = 0.52 \text{ g cm}^{-3}$ ) <sup>[57]</sup>
Critical T [K]	690 (explosion in 250 ms) <sup>[63]</sup>
Trauzl test [cm <sup>3</sup> , % TNT]	10 g AN, slight confinement, can be completely detonated by a no. 8 blasting cap, ~166 cc <sup>[17]</sup> , 10 g AN slight confinement incomplete detonation with no. 6 blasting cap and no detonation with smaller blasting caps <sup>[17]</sup> , Only partial detonation occurred with AN of maximum $\rho$ (from melting then solidifying) <sup>[17]</sup> , 225 cc (for complete detonation, cf. 300 cc for TNT) <sup>[17]</sup> , 165 cc (for incomplete detonation) <sup>[17]</sup> , 55% TNT <sup>[17,59]</sup> , 75% TNT <sup>[19,26]</sup> , 56% TNT <sup>[3]</sup> , 40.0 (Trauzl test number, 6.0 g sample, 3 dram vial with plastic cap with opening for no. 8 blasting cap) <sup>[69]</sup> , 200 mL/10 g (small crystals of 0.15–0.4 mm) <sup>[70]</sup> , 135 mL/10 g (long rhombic crystals, 3 cm long) <sup>[70]</sup> , 15 mL/10 g (large pieces produced by breaking after melting and solidification) <sup>[70]</sup>

Brisance	54% TNT (lead cylinder compression test) <sup>[59]</sup> , 54% TNT (for sample with $\rho = 1.3 \text{ g cm}^{-3}$ ) <sup>[26]</sup>																																							
Sand test [g]	Incomplete detonation <sup>[26]</sup> , only partial explosion occurs even if tetryl or RDX booster charge used <sup>[26]</sup> , larger charges can be detonated by tetryl booster charge <sup>[26]</sup> , nil (200 g bomb) <sup>[3]</sup>																																							
Ballistic mortar test	56% TNT <sup>[7]</sup> , 79% TNT <sup>[19]</sup> , 79% TNT (@ 1.0 g cm <sup>-3</sup> ) <sup>[26]</sup> , 58% PA (ballistic mortar Mk. IIId test) <sup>[74]</sup>																																							
Initiation efficiency	0.20 g minimum detonating charge of LA <sup>[7]</sup> , 0.25 g minimum detonating charge of tetryl <sup>[7]</sup> , more difficult to detonate or explode than any of the standard military explosives <sup>[59]</sup> , no. 8 blasting cap does not cause complete detonation if AN unconfined <sup>[26]</sup> , easier to initiate molten AN than solid AN <sup>[26]</sup> , dry AN easier to initiate than moist AN <sup>[26]</sup> , sensitivity to initiation decreases with increasing loading density and @ $\rho > 0.9 \text{ g cm}^{-3}$ , 1–3 lb charges of AN cannot be completely detonated by booster charges <sup>[26]</sup> , larger charges cannot be completely detonated @ $\rho > 1.1 \text{ g cm}^{-3}$ <sup>[26]</sup>																																							
US NOL gap test	Gap value <0 cm for 1.65 g cm <sup>-3</sup> , pressed AN <sup>[18]</sup>																																							
LSGT [cm]	All charges are conditioned and fired at 25 °C unless otherwise indicated, data from <sup>[66]</sup> :																																							
	<table border="1"> <thead> <tr> <th rowspan="2">Material</th> <th rowspan="2"><math>\rho</math> (g/cm<sup>3</sup>)</th> <th rowspan="2">% TMD</th> <th colspan="3">90% point</th> <th rowspan="2">Particle size (μm)</th> </tr> <tr> <th>Cards</th> <th>Type of test</th> <th>kbar</th> </tr> </thead> <tbody> <tr> <td rowspan="4">AN prills</td> <td>0.86</td> <td>49.6</td> <td>53 (packed by hand)</td> <td>Extended test</td> <td>77</td> <td>2,000</td> <td>No det.</td> </tr> <tr> <td>1.06</td> <td>62.4</td> <td>35 (packed by hand)</td> <td>Extended test</td> <td>90</td> <td>2,000</td> <td>No det.</td> </tr> <tr> <td>1.13</td> <td>65.5</td> <td>31 (hydraulic press)</td> <td></td> <td>94</td> <td>2,000</td> <td>No det.</td> </tr> <tr> <td>1.20</td> <td>69.6</td> <td>1 ± 1 (hydraulic press)</td> <td>Extended test</td> <td>175</td> <td>2,000</td> <td>No det.</td> </tr> </tbody> </table>	Material	$\rho$ (g/cm <sup>3</sup> )	% TMD	90% point			Particle size (μm)	Cards	Type of test	kbar	AN prills	0.86	49.6	53 (packed by hand)	Extended test	77	2,000	No det.	1.06	62.4	35 (packed by hand)	Extended test	90	2,000	No det.	1.13	65.5	31 (hydraulic press)		94	2,000	No det.	1.20	69.6	1 ± 1 (hydraulic press)	Extended test	175	2,000	No det.
Material	$\rho$ (g/cm <sup>3</sup> )				% TMD	90% point			Particle size (μm)																															
		Cards	Type of test	kbar																																				
AN prills	0.86	49.6	53 (packed by hand)	Extended test	77	2,000	No det.																																	
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	1.20	69.6	1 ± 1 (hydraulic press)	Extended test	175	2,000	No det.																																	
3 s explosion $T$ [°C]	325 <sup>[17]</sup>																																							
5 s ignition $T$ [°C]	465 (ignites) <sup>[3,7,18]</sup>																																							
5 s explosion $T$ [°C]	No explosion <sup>[26]</sup>																																							
Explosion $T$ [°C]	AN hermetically confined explodes on rapid heating >200 °C <sup>[40]</sup> , AN confined hermetically undergoes explosive dec. @ 260–280 °C <sup>[40]</sup> , 325 (deflagration) <sup>[26]</sup>																																							
Ignition $T$ [°C]	465 <sup>[56]</sup> , 465 (unconfined sample) <sup>[59]</sup> , 260–360 (confined sample) <sup>[59]</sup>																																							

Flash point [°C]	500 <sup>[59]</sup>																
Thermal stability	N content decreased from 33.3% to 32.9% after storage @ 80 °C for 2 weeks <sup>[17]</sup> , 0 mol gas formed per mole AN in 22 h @ 120 °C <sup>[24]</sup> , 0 mol gas formed per mole AN in 72 h <sup>[24]</sup> , @ 220 °C, 0.88 mol gas formed per mole AN in 22 h. <sup>[24]</sup> , 0.9 mol gas formed per mole AN in 72 h <sup>[24]</sup> , @ 320 °C, 0.89 mol gas formed per mole AN in 22 h. <sup>[24]</sup> , 0.9 mol gas formed per mole AN in 72 h <sup>[24]</sup> , very stable in storage up to 150 °C, although slight dec. may occur <sup>[59]</sup> , no appreciable dec. after 100 days @ 100 °C, dec. appears to begin @ 170 °C <sup>[59]</sup> , very stable in storage @ temperatures as high as 150 °C (slight sublimation may occur under certain conditions) <sup>[3]</sup>																
100 °C heat test [% mass loss]	0.74% mass loss in first 48 h <sup>[7,17]</sup> , 0.13% mass loss in second 48 h <sup>[7,17]</sup> , no explosion in 100 h <sup>[7,17]</sup> , 0.1% mass loss in first 48 h <sup>[26]</sup> , 0.0% mass loss in second 48 h <sup>[26]</sup>																
75 °C heat test [% mass loss]	0.0 in 48 h <sup>[7]</sup>																
Vacuum stability test [cm <sup>3</sup> /h]	0.1–1.0 cc gas evolved from 5 g AN in 40 h @ 120 °C <sup>[17]</sup> , 0.2–0.3 cc gas evolved from 5 g AN in 40 h @ 150 °C <sup>[17]</sup> , no dec. after heating @ 100 °C for 100 days <sup>[26]</sup> , 0.3 cc/40 h @ 100 °C <sup>[7]</sup> , 0.3 cc/40 h @ 120 °C <sup>[7]</sup> , 0.3 cc/40 h @ 150 °C <sup>[7]</sup>																
C <sub>p</sub> [J mol K <sup>-1</sup> ]	137.6 <sup>[32,47]</sup> , 139.3 <sup>[34,49,52]</sup>																
Dissociation pressures (mm Hg / @ °C)	3.25/@ 188.2 <sup>[17]</sup> , 7.45/@ 205.1 <sup>[17]</sup> , 11.55/@ 215.9 <sup>[17]</sup> , 15.8/@ 223.1 <sup>[17]</sup> , 27.0/@ 236.7 <sup>[17]</sup> , 41.0/@ 249.1 <sup>[17]</sup>																
Vapor pressure [atm @ °C]	12 ppb (v/v) @ 25 °C <sup>[20]</sup> , no clear dependence of the vapor pressure on the humidity was observed <sup>[20]</sup> , $5.98 \times 10^{-4}$ Pa @ 25 °C <sup>[21]</sup> , 7.4 mm Hg @ 205 °C <sup>[54]</sup> Vapor pressure values from <sup>[7]</sup> : <table border="1"> <thead> <tr> <th>T(°C)</th> <th>Vapor pressure (mm Hg)</th> <th>T(°C)</th> <th>Vapor pressure (mm Hg)</th> </tr> </thead> <tbody> <tr> <td>188</td> <td>3.25</td> <td>223</td> <td>15.80</td> </tr> <tr> <td>205</td> <td>7.45</td> <td>237</td> <td>27.0</td> </tr> <tr> <td>216</td> <td>11.55</td> <td>249</td> <td>41.0</td> </tr> </tbody> </table>	T(°C)	Vapor pressure (mm Hg)	T(°C)	Vapor pressure (mm Hg)	188	3.25	223	15.80	205	7.45	237	27.0	216	11.55	249	41.0
T(°C)	Vapor pressure (mm Hg)	T(°C)	Vapor pressure (mm Hg)														
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205	7.45	237	27.0														
216	11.55	249	41.0														
Volatility	Dec. @ 210 °C <sup>[7]</sup>																
Burn rate [mm/s]	Will explode if involved in a fire if mixed with combustible material <sup>[67]</sup>																

Solubility [g/mL]	<p>Solubility values (g AN/100 g solvent) from<sup>[7]</sup>:</p> <table border="1"> <thead> <tr> <th colspan="2">H<sub>2</sub>O</th> <th colspan="2">EtOH</th> <th colspan="2">Acetic acid</th> </tr> <tr> <th>T (°C)</th> <th>%</th> <th>T (°C)</th> <th>%</th> <th>T (°C)</th> <th>%</th> </tr> </thead> <tbody> <tr> <td>0</td> <td>118</td> <td>20</td> <td>2.5</td> <td>16.6</td> <td>0.0</td> </tr> <tr> <td>20</td> <td>192</td> <td>40</td> <td>5</td> <td>27.0</td> <td>0.39</td> </tr> <tr> <td>40</td> <td>297</td> <td>60</td> <td>7.5</td> <td>80.9</td> <td>5.8</td> </tr> <tr> <td>60</td> <td>421</td> <td>78</td> <td>10.5</td> <td>101.0</td> <td>20.7</td> </tr> <tr> <td>80</td> <td>580</td> <td></td> <td></td> <td>120.0</td> <td>125</td> </tr> <tr> <td>100</td> <td>871</td> <td></td> <td></td> <td></td> <td></td> </tr> </tbody> </table> <p>~20–25 g/100 g pyridine @ 25 °C<sup>[7]</sup>, highly H<sub>2</sub>O soluble<sup>[32,47]</sup>, 63 g AN dissolves in 100 g N,N-DMF @ 60 °C<sup>[32]</sup>, soluble in methanol (14% AN is dissolved @ 18.5 °C)<sup>[38]</sup>, soluble in ethanol<sup>[38]</sup>, 66 g/100 g H<sub>2</sub>O @ 20 °C<sup>[54]</sup></p> <p>Solubility of AN in H<sub>2</sub>O<sup>[38]</sup>:</p> <table border="1"> <thead> <tr> <th>T (°C)</th> <th>Solubility (%)</th> <th>T (°C)</th> <th>Solubility (%)</th> </tr> </thead> <tbody> <tr> <td>20</td> <td>66.1</td> <td>100</td> <td>91.0</td> </tr> <tr> <td>40</td> <td>73.3</td> <td>120</td> <td>94.7</td> </tr> <tr> <td>60</td> <td>80.2</td> <td>140</td> <td>97.4</td> </tr> <tr> <td>80</td> <td>85.9</td> <td>160</td> <td>99.4</td> </tr> </tbody> </table> <p>Soluble in alcohol, acetic acid, nitric acid<sup>[54]</sup>, very soluble in water<sup>[56]</sup>, slightly soluble in EtOH<sup>[56]</sup>, soluble in warm MeOH<sup>[56]</sup>, soluble in H<sub>2</sub>O, EtOH, MeOH and other organic solvents containing –OH or –NH groups<sup>[59]</sup></p> <p>Solubility of AN in DMF (g/100 g DMF) after 5 min stirring<sup>[62]</sup>: 47 @ 0 °C<sup>[62]</sup>, 54 @ 25 °C<sup>[62]</sup></p> <p>Very soluble in water – water dissolves 1.2× its weight @ 0 °C and 11× its weight @ 100 °C<sup>[67]</sup>, 210 g/100 g H<sub>2</sub>O @ 25 °C<sup>[71]</sup>, 1 g dissolves in 0.5 mL water<sup>[73]</sup>, 1 g dissolves in 0.1 mL boiling water<sup>[73]</sup>, 1 g dissolves in 20 mL EtOH<sup>[73]</sup>, 1 g dissolves in 8 mL MeOH<sup>[73]</sup></p>	H <sub>2</sub> O		EtOH		Acetic acid		T (°C)	%	T (°C)	%	T (°C)	%	0	118	20	2.5	16.6	0.0	20	192	40	5	27.0	0.39	40	297	60	7.5	80.9	5.8	60	421	78	10.5	101.0	20.7	80	580			120.0	125	100	871					T (°C)	Solubility (%)	T (°C)	Solubility (%)	20	66.1	100	91.0	40	73.3	120	94.7	60	80.2	140	97.4	80	85.9	160	99.4
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Hygroscopicity	Extremely hygroscopic <sup>[3]</sup> , very hygroscopic <sup>[32,38,47,60]</sup> , usually used as prills because of its strong H <sub>2</sub> O affinity <sup>[32,47]</sup> , highly hygroscopic, becomes liq. in moist air <sup>[38]</sup> , hygroscopic point of 62% <sup>[62]</sup> , hygroscopic but does not form hydrates <sup>[54]</sup> , absorbs moisture readily <sup>[56]</sup> , hygroscopic crystals <sup>[59]</sup> , extremely hygroscopic <sup>[59]</sup> , extreme @ 30 °C, 90% RH <sup>[7]</sup> , critical humidity = 66% RH @ 20 °C <sup>[72]</sup> , hygroscopic deliquescent crystals <sup>[73]</sup>																																																																				

Compatibility	In the presence of moisture it reacts with copper, iron, steel, brass, lead and cadmium. <sup>[7,56]</sup> In the presence of moisture it reacts with Cu to form a highly impact sensitive compound; therefore, copper, brass or bronze should not be used <sup>[59]</sup> ; reacts with and corrodes iron, steel, lead, cadmium and zinc <sup>[59]</sup> ; materials suitable for protective coatings for containers containing AN compositions are polyvinyl chloride and epoxy resins <sup>[59]</sup> ; incompatible with acid-proof black paint, shellac, baked oil and rubber paints <sup>[59]</sup> ; sensitivity of AN to heat is increased by the presence of organic materials and therefore organic or flammable materials should not be stored with or adjacent to AN <sup>[59]</sup> ; dec. by strong alkalis or sulfuric acid <sup>[7,59]</sup> ; dec. by strong alkalis and conc. sulfuric acid <sup>[26]</sup> ; reacts with Cu in the presence of moisture <sup>[26]</sup> ; incompatible with brass or bronze <sup>[26]</sup> ; sensitivity to heat increases by the presence of Cu, iron, Al, Zn, chromium oxide or chromium nitrate <sup>[26]</sup> ; sensitivity to heat decreased by addition of powdered limestone, Kieselguhr and clay residue <sup>[26]</sup> ; in the presence of moisture reacts with Cu to form an extremely sensitive compound <sup>[3]</sup> ; corrodes Fe, steel, brass, lead and cadmium <sup>[3]</sup> ; incompatible with Cu or Cu alloys and should not be brought into contact with Cu or Cu alloys since it can form unstable compounds <sup>[67]</sup> ; promotes corrosion of Fe and steel <sup>[67]</sup> ; attacks Pb <sup>[67]</sup> ; can be handled in Al or stainless steel equipment <sup>[67]</sup>																				
Heat of fusion [J/g]	76.7 <sup>[54]</sup> , 18.23 cal/g <sup>[7,26]</sup>																				
Heat of sublimation [kcal/mol]	Latent heat of sublimation = 41.8 @ 25 °C <sup>[26]</sup>																				
Flame T [°C]	1,500 (est.) <sup>[54]</sup>																				
Coefficient of thermal expansion [%/°C]	$9.82 \times 10^{-4}$ @ 20 °C <sup>[54]</sup>																				
Specific heat [J/mol]	0.189 cal/g/°C @ -150 °C <sup>[7]</sup> , 0.330 cal/g/°C @ -100 °C <sup>[7]</sup> , 0.364 cal/g/°C @ -50 °C <sup>[7]</sup> , 0.397 cal/g/°C @ 0 °C <sup>[7]</sup> , 0.414 cal/g/°C @ 50 °C <sup>[7]</sup> , 0.428 cal/g/°C @ 100 °C <sup>[7]</sup> , 1.72 (from 0 to 31 °C) <sup>[54]</sup>  Values from <sup>[26]</sup> :																				
	<table border="1"> <thead> <tr> <th>T(°C)</th> <th>Specific heat (cal/g °C)</th> <th>T(°C)</th> <th>Specific heat (cal/g °C)</th> </tr> </thead> <tbody> <tr> <td>-200</td> <td>0.07</td> <td>-50</td> <td>0.37</td> </tr> <tr> <td>-150</td> <td>0.19</td> <td>0</td> <td>0.40</td> </tr> <tr> <td>-100</td> <td>0.30</td> <td>50</td> <td>0.414</td> </tr> <tr> <td>-80</td> <td>0.35</td> <td>100</td> <td>0.428</td> </tr> </tbody> </table>	T(°C)	Specific heat (cal/g °C)	T(°C)	Specific heat (cal/g °C)	-200	0.07	-50	0.37	-150	0.19	0	0.40	-100	0.30	50	0.414	-80	0.35	100	0.428
T(°C)	Specific heat (cal/g °C)	T(°C)	Specific heat (cal/g °C)																		
-200	0.07	-50	0.37																		
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Heat of dec. [kJ/mol]	316 (DSC @ 20 °C/min) <sup>[55]</sup> , 323 cal/g <sup>[59]</sup> , 961 J/g (DSC) <sup>[74]</sup>																				

Rifle bullet impact test	100% unaffected in trials <sup>[7]</sup> , unaffected <sup>[59]</sup> , no explosions <sup>[26]</sup>
Thermal conductivity [cal/s/cm/°C]	$2.9\text{--}3.9 \times 10^{-4}$ <sup>[7]</sup>
Hardness	1.1 (Mohs' scale, scratch hardness) <sup>[26]</sup>
pH	5.43 (0.1 M soln. in water) <sup>[73]</sup>
UN princess incendiary spark test	Failed to ignite <sup>[74]</sup>
High-pressure autoclave test	$F$ -value = 14.3 J/g <sup>[74]</sup>
Detonability	BAM 50/60 tube test (detonator + 50 g RDX): fragmented length = 50 cm (split), result = partial <sup>[74]</sup>
Koenen test	Critical diameter = 1.0 mm, result = low <sup>[74]</sup>
Dutch pressure vessel test	Critical diameter = 1.0 mm, result = low <sup>[74]</sup>
Thermal explosion vessel test	Max. rate × max. pressure = 0.16 MPa <sup>2</sup> /s, result = low <sup>[74]</sup>

ARC experiments<sup>[43]</sup>:

Mass of AN (dry) = 1.001 g, closed system,  $p_i = 0.1$  MPa, air,  $T_0 = 200 \pm 5$  °C  
(runaway exo. dec.)<sup>[43]</sup>

Mass of AN (dry) = 3.001 g, closed system,  $p_i = 0.1$  MPa, air,  $T_0 = 199 \pm 7$  °C  
(runaway exo. dec.)<sup>[43]</sup>

Mass of AN (dry) = 3.001 g, open system,  $p_i = 0.1$  MPa, air,  $197 \pm 5$  °C  
(weak exotherm,  $R_{\max} = 0.04$  °C min<sup>-1</sup>), 217 ± 5 °C (runaway)<sup>[43]</sup>

Adiabatic Dewar calorimeter (ADC) experiments<sup>[43]</sup>:

AN (dry), mass = 99.9 g, closed system,  $T_0 = 192 \pm 5$  °C<sup>[43]</sup>

AN (dry), mass = 100.9 g, open system,  $T_0 = 187 \pm 10$  °C (start of self-heating), 219 ± 5 °C<sup>[43]</sup>

	AN-I <sup>[15]</sup>	AN-II <sup>[15]</sup>	AN-III <sup>[15]</sup>	AN-IV <sup>[15]</sup>	AN-V <sup>[15]</sup>
	(ε-)	(δ-)	(ν-)	(β-)	
Chemical formula	H <sub>4</sub> N <sub>2</sub> O <sub>3</sub>				
Molecular weight [g mol <sup>-1</sup> ]	80.04	80.04	80.04	80.04	80.04

Crystal system	Cubic	Tetragonal	Orthorhombic	Orthorhombic	Orthorhombic
Space group	$P\bar{m}\bar{3}m$ (no. 221)	$P\bar{4}2_1m$ (no. 113) $P4/mbm$ (no. 127)	$Pnma$ (no. 53)	$Pmm$ (no. 47)	$Pccn$ (no. 56)
$a$ [Å]	4.366	5.7193	7.7184	5.745	7.983
$b$ [Å]	4.366	5.7193	5.8447	5.438	7.972
$c$ [Å]	4.366	4.9326	7.1624	4.942	9.832
$\alpha$ [°]	90	90	90	90	90
$\beta$ [°]	90	90	90	90	90
$\gamma$ [°]	90	90	90	90	90
$V$ [Å <sup>3</sup> ]	83.2245	161.347	323.108	154.395	555.07
$Z$	1	2	4	2	8
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.59706	1.64756	1.64545	1.72175	1.91563
$T$ [°C]	150	82	45	22	<255 K

	AN-IV <sup>[8,27,28]</sup>	AN-IV <sup>[29]</sup>	AN-V <sup>[30]</sup>	AN-I <sup>[8]</sup>	AN-II <sup>[8]</sup>	AN-III
	(β-)	(neutron diffraction)	(α-)	(ε-)	(δ-)	(γ-)
Chemical formula	H <sub>4</sub> N <sub>2</sub> O <sub>3</sub>					
Molecular weight [g mol <sup>-1</sup> ]	80.04	80.04	80.04	80.04	80.04	80.04
Crystal system	Orthorhombic	Orthorhombic	Tetragonal	Cubic	Tetragonal	Orthorhombic
Space group	$P4mmn$	$Pmmn$	$P42$ (no. 77)		$P421m$ or $P4mbm$	
$a$ [Å]	5.724		7.98	4.40	5.72	7.14
$b$ [Å]	5.455		7.98	4.40	5.72	7.65
$c$ [Å]	4.945		9.78	4.40	4.93	5.83
$\alpha$ [°]	90	90	90	90	90	90
$\beta$ [°]	90	90	90	90	90	90
$\gamma$ [°]	90	90	90	90	90	90
$V$ [Å <sup>3</sup> ]						
$Z$	2	2	8	1		

$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]						
T [K]			-150 °C			42 °C

Crystallographic data and stability ranges of AN phases<sup>[36, 43]</sup>:

Phase/ property	V <sup>[36,43]</sup>	IV <sup>[36,43,50]</sup>	III <sup>[36,43]</sup>	II <sup>[36,43]</sup>	I <sup>[36,43]</sup>
Crystal system	Orthorhombic	Orthorhombic	Orthorhombic	Tetragonal	Cubic
Space group	Pccn	Pmmn	Pnma	P4/mmbm	Pm3m
Z	8	2	4	2	1
Lattice parameters	$a = 7.943 \text{ \AA}$ $b = 7.972 \text{ \AA}$ $c = 9.832 \text{ \AA}$	$a = 5.745 \text{ \AA}$ $b = 5.438 \text{ \AA}$ $c = 4.942 \text{ \AA}$	$a = 7.7184 \text{ \AA}$ $b = 5.8447 \text{ \AA}$ $c = 7.1624 \text{ \AA}$	$a = 5.7193 \text{ \AA}$ $c = 4.9326 \text{ \AA}$	$a = 4.366 \text{ \AA}$
T <sub>measurement</sub> (K)	173 (-100 °C)	295 (22 °C)	318 (45 °C)	355 (82 °C)	423 (150 °C)
Stability range (K)	Humid <255 (less than -18 °C), Dry <255 (less than -18 °C)	Humid 255–305 (-18–32 °C), Dry 255–328 (-18–32 °C)	Humid 305–357 (32–84 °C), Dry –	Humid 357–398 (84–125 °C), Dry <328–398 (55–125 °C)	Humid >398 (>125 °C), Dry >398 (>125 °C)

Phase I: cubic, 170–125 °C<sup>[54]</sup>

Phase II: tetragonal, 125–84 °C<sup>[54]</sup>

Phase III: orthorhombic, 84–32 °C<sup>[54]</sup>

Phase IV: orthorhombic, 32 to -16 °C<sup>[54]</sup>

Phase V: tetragonal, less than -16 °C<sup>[54]</sup>

Volume changes of AN phase transitions<sup>[36]</sup>:

Phase transition	T (K)	Vol. change (Å <sup>3</sup> )	% vol. change
II → I	404	1.88	2.3
III → II	365	1.37	1.7
IV → II	323	1.61	2.0
II → V	317	0.23	0.3
IV → III	314	2.94	3.7
V → IV	272	2.20	2.8
IV → V	224	2.49	3.2

Crystal modifications of AN<sup>[26]</sup>:

Form	Crystal system	Range (°C)
Liquid		>169.6
I epsilon	Regular (cubic) (isometric)	125.0–169.6
II delta	Rhombohedral or tetragonal	84.1–125
III gamma	Orthorhombic	32.3–84.1
IV beta	Orthorhombic	–18–32.2
V alpha	Tetragonal	–18 to –150

Effects of transformation between AN crystalline modifications (*Hendricks et al.*)<sup>[38]</sup>:

Crystalline form of AN	T (°C)	Change of vol. (cm <sup>3</sup> /g)	Thermal effect (cal/g)
I → II	125.2	–0.013	+11.9
II → III	84.2	+0.008	+5.3
III → IV	32.1	–0.002	+5.0
IV → V	–18	+0.016	+1.6

Volume variation of the different AN phases<sup>[51]</sup>:

Modification	Volume variation (%)	Volume variation (cm <sup>3</sup> /g)
I → II	–2.2	Approx. $-1.4 \times 10^{-2}$
II → III	+1.3	Approx. $0.8 \times 10^{-2}$
III → IV	–3.6	Approx. $-2.2 \times 10^{-2}$
IV → V	+2.4	Approx. $1.7 \times 10^{-2}$
II → V	–2.3	Approx. $-1.4 \times 10^{-2}$

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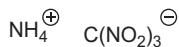
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## Ammonium nitroformate

Name [German, acronym]: Ammonium trinitromethanide, [ammonium-nitroformat, ammoniumtrinitromethanid, ANF]

Main (potential) use: oxidizer

Structural formula:



	ANF		
Formula	$\text{CH}_4\text{N}_4\text{O}_6$		
Molecular mass [g mol <sup>-1</sup> ]	168.08		
Appearance at RT			
IS [J]	3 (BAM) <sup>[1]</sup>		
FS [N]	96 <sup>[1]</sup>		
ESD [J]			
N [%]	33.3		
$\Omega(\text{CO}_2)$ [%]	+19.0		
$T_{\text{m.p.}}$ [°C]			
$T_{\text{dec.}}$ [°C]	116 (DSC @ 2 °C/min) <sup>[1]</sup> , 112 (TGA @ 1 °C/min) <sup>[4]</sup>		
$\rho$ [g cm <sup>-3</sup> ]	1.910 (cryst., @ 100 K) <sup>[1]</sup>		
Heat of formation	-35.9 kcal mol <sup>-1</sup> <sup>[1]</sup> , -47.3 kcal mol <sup>-1</sup> <sup>[2]</sup>		
Heat of combustion	-1,108.6 cal/g <sup>[2]</sup>		
	Calcd. (EXPLO5 5.02)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^\circ$ [kJ kg <sup>-1</sup> ]	4,328 <sup>[1]</sup>		
$T_{\text{ex}}$ [K]	3,575 <sup>[1]</sup>		
$p_{\text{C}_1}$ [kbar]	312 <sup>[1]</sup>		
VoD [m s <sup>-1</sup> ]	8,532 (@ 1.910 g cm <sup>-3</sup> ) <sup>[1]</sup>		
$V_0$ [L kg <sup>-1</sup> ]	800 <sup>[1]</sup>		
Trauzl test [cm <sup>3</sup> , % TNT]	-, 128% <sup>[3]</sup>		
Sand test [g]			
Ballistic mortar test			

LSGT [cm]	
SSGT [cm]	
5 s explosion $T$ [°C]	
100 °C heat test [% mass loss]	
Vacuum stability test [cm <sup>3</sup> /h]	
Vapor pressure [atm @ °C]	
Burn rate [mm/s]	
Solubility [g/mL]	

	ANF <sup>[1]</sup>
Chemical formula	CH <sub>4</sub> N <sub>4</sub> O <sub>6</sub>
Molecular weight [g mol <sup>-1</sup> ]	168.08
Crystal system	Tetragonal
Space group	P4 <sub>1</sub> 2 <sub>1</sub> 2 (no. 92)
$a$ [Å]	6.7617(1)
$b$ [Å]	6.7617(1)
$c$ [Å]	12.7877(4)
$\alpha$ [°]	90
$\beta$ [°]	90
$\gamma$ [°]	90
$V$ [Å <sup>3</sup> ]	584.66(2)
$Z$	4
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.910
$T$ [K]	100

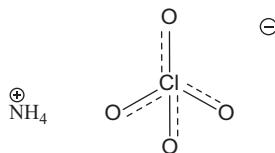
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## Ammonium perchlorate

Name [German, acronym]: Ammonium perchlorate [ammoniumperchlorat, ammonperchlorat, AP, APC]

Main (potential) use: Oxidizer in composite propellants<sup>[1, 65]</sup> pyrotechnics, projectile filler, ingredient in flares, igniters, incendiaries, smoke-generating compositions, component of perchlorate high explosives<sup>[34]</sup>, constituent of solid rocket fuels<sup>[34]</sup>, component of primer, pyrotechnic and propellant compositions<sup>[46]</sup>, detonating and pyrotechnic compositions<sup>[48]</sup>, oxidizer in some firework compositions<sup>[65]</sup>, explosives, pyrotechnic compositions, jet and rocket propellants<sup>[67]</sup>

Structural formula:



	APC
Formula	$\text{NH}_4\text{ClO}_4$
Molecular mass [g mol <sup>-1</sup> ]	117.49
Appearance at RT	White powder <sup>[46]</sup> , colorless crystals <sup>[48]</sup> , colorless rhombic crystals <sup>[62]</sup> , orthorhombic crystals <sup>[67]</sup> , white crystals <sup>[68]</sup>
IS [J]	15 <sup>[1]</sup> , 15–25 Nm <sup>[5]</sup> , 5 <sup>[6]</sup> , 13.15 (67 cm, 2 kg mass, 20 mg sample, B. M.) <sup>[7]</sup> , 11.97 (24 in, 24 mg sample, 2 kg mass, P.A.) <sup>[7]</sup> , 15 <sup>[11]</sup> , $H_{50\%}$ = 107 cm (NOL apparatus) <sup>[18]</sup> , $H_{50\%}$ = 91 cm (2 kg mass, B.M.) <sup>[18]</sup> , $H_{50\%}$ = 24 in (2 kg mass, P.A.) <sup>[18]</sup> , $H_{50\%}$ = 100 cm (2 kg mass, B.M.) <sup>[20]</sup> , 46 in (5 lb mass, unspecified test) <sup>[20]</sup> , 13.7 (BAM, Julius-Peters) <sup>[29]</sup> , $E_{50}$ = 7.9 (raw, ultra-fine AP) <sup>[33]</sup> , explodes on 10 kg dropped 15 cm <sup>[34]</sup> , 50 cm drop of 5 kg mass caused explosions in ~50% of trials <sup>[35]</sup> , 4.7 kg (steel on steel impact) <sup>[49]</sup> , 1.9 kg (@ 160 °C, steel on steel impact) <sup>[49]</sup> , $H_{50}$ = 47.9 cm (nonspherical AP) <sup>[63]</sup> , $H_{50}$ = 63.1 cm (spherical AP) <sup>[63]</sup> , limiting impact energy = 5 J (BAM) <sup>[69]</sup> , $H_{50}$ = 55 cm (design no. 3 apparatus) <sup>[72]</sup> , $H_{50}$ = 46 cm (design no. 5 apparatus) <sup>[72]</sup> , $H_{50}$ = 38 cm (design no. 11 apparatus, 2.5 kg hammer) <sup>[72]</sup> , $H_{50}$ = 36 cm (design no. 12 apparatus, 48 units, cf. TNT = 100 units) <sup>[72]</sup>

	% explosions in instrument no. 4, K-44-2 drop hammer 10 kg load, 25 cm drop height, two different locations for charge <sup>[70]</sup> :
Weight (mg)	
Centrally located	
2	10
48	84
Uniformly located	
2	10
48	84
mg	
—	
4	
0	
%	
FS [N]	>320 <sup>[5]</sup> , >363 <sup>[6]</sup> , >100 <sup>[11]</sup> , P/% = 94 (raw, ultra-fine AP) <sup>[33]</sup> , 30% @ 353 (BAM, Julius-Peters) <sup>[29]</sup> , snaps with steel shoe (friction pendulum test) <sup>[7]</sup> , unaffected by fiber shoe (friction pendulum test) <sup>[7]</sup> , limiting load ≥ 363 N (BAM) <sup>[69]</sup>
ESD [J]	>5 <sup>[18]</sup> , ≥ 726 mJ <sup>[29]</sup> , $E_{50\%} = 0.41 \pm 0.02$ (AP = 90 μm, Bruceton eq.) <sup>[37]</sup> , $E_{50\%} = 0.53 \pm 0.05$ (AP = 200 μm, Bruceton eq.) <sup>[37]</sup> , > 156 mJ (closed container) <sup>[41]</sup> , > 156 mJ (open container) <sup>[41]</sup>
N [%]	11.92
Ω(CO <sub>2</sub> ) [%]	+27.2
$T_{\text{phase transitions}}$ [°C]	Orthorhombic @ 25 °C <sup>[20,34]</sup> , cubic > 240 °C <sup>[20,34]</sup> , crystalline transition rhombic → cubic @ 240 °C <sup>[62]</sup> , DTA (15 °C/min): 235–244 (endo) <sup>[24]</sup> , 240 (rhombic – cubic transition $T$ ) <sup>[24]</sup> , ~240 (orthorhombic → cubic) <sup>[53,59]</sup> , -190 (probable first order polymorphic transition) <sup>[53]</sup>  Data from <sup>[58]</sup> : ~240 (long assumed first-order transition from orthorhombic cubic. Changes in dec. rate @ 240 °C attributed to formation of cubic structure) <sup>[58]</sup> . However, this is questioned by investigations (Aerojet Laboratories) on crystal transitions using X-ray diffraction which showed irreversible transition @ 240 °C, which is distinct from the reversible orthorhombic cubic transition that occurs at higher $T$ . No structural change observed @ 240 °C using X-ray diffraction, but differences in intensity in diffractograms were observed. Cubic structure observed @ 260 °C disappeared on cooling with a return to diffraction pattern observed at 240 °C. It is suggested that abnormal dec. behavior @ ~240 °C is due to an irreversible second-order phase transition <sup>[58]</sup> . Maximum rate of dec. occurred slightly below 240 °C, but continuously decreasing dec. rate up to $T$ ~250 °C, which would be expected for second-order phase transition. Second-order transitions were observed for other NH <sub>4</sub> <sup>+</sup> salts and were known to cause modification of dec. behavior of solid. <sup>[58]</sup>

	<p>Heating single crystals and photographing the crystals: crystal no. 1 heated @ 190 °C for three separate intervals of each 30 min; crystal no. 2 heated @ 220 °C for three separate intervals of 15 min each and crystal no. 3 heated @ 250 °C for three separate intervals of 3 min each. Crystal no. 1 showed the formation of amorphous layer on surface which loosened from crystal surface, formed clumps which then formed single rhombic crystallites – at the end of heating periods no amorphous material was left and only rhombic crystals remained; crystal no. 2 showed the same behavior as crystal no. 1; however, it occurred more quickly, but at the end of heating degeneration of some crystallites was observed; crystal no. 3 showed no crystallite growth that was observed for crystal no. 1 or 2, only darkening and deterioration of the surface of the original crystal was observed in which it turned milky and had a poor surface structure.<sup>[58]</sup></p> <p>(see additional, detailed section later)</p>										
$T_{m.p.}$ [°C]	<p>&gt;300<sup>[2]</sup>, &gt;220 (with dec.)<sup>[8]</sup>, dec. @ 440 without melting<sup>[20]</sup>, 243.7 (endo, DSC, ultra-fine AP)<sup>[33]</sup>, 235 (with dec.)<sup>[11]</sup>, dec.<sup>[29]</sup>, 220.1 (DSC)<sup>[42]</sup>, dec. before melting<sup>[46,48]</sup>, does not melt but begins to sublime with slow dec. @ 130 °C<sup>[65]</sup>, &lt;240 °C (orthorhombic)<sup>[8]</sup>, &gt;240 °C (cubic, <math>\rho = 1.71 \text{ g cm}^{-3}</math>)<sup>[8]</sup></p> <p>Analytical-grade AP, &gt;99% purity, average particle size = 30–40 µm, TG/DSC-MS-FTIR, 2 mg sample, alumina crucible with prehole in lid, Ar<sup>[45]</sup>:</p> <table border="1" style="margin-left: auto; margin-right: auto;"> <thead> <tr> <th>Heating rate (K/min)</th> <th>Max. endothermic peak <math>T</math> (°C)</th> </tr> </thead> <tbody> <tr> <td>5</td> <td>244</td> </tr> <tr> <td>10</td> <td>247</td> </tr> <tr> <td>15</td> <td>247</td> </tr> <tr> <td>20</td> <td>247</td> </tr> </tbody> </table> <p>(see additional, detailed section later)</p>	Heating rate (K/min)	Max. endothermic peak $T$ (°C)	5	244	10	247	15	247	20	247
Heating rate (K/min)	Max. endothermic peak $T$ (°C)										
5	244										
10	247										
15	247										
20	247										
$T_{dec.}$ [°C]	<p>320<sup>[1]</sup>, 389 (DSC @ 5 K/min)<sup>[6]</sup>, DTA: phase transition @ 240, 300 (LT<sub>dec.</sub>), 400 (HT<sub>dec.</sub>)<sup>[12]</sup>, 295.56 (onset, LTD peak), 311.3 (LTD peak) (DSC)<sup>[32]</sup>, 419 (onset, HTD peak), 439 (HTD peak) (DSC)<sup>[32]</sup>, 441.8 (exo, DSC, HTD, ultra-fine AP)<sup>[33]</sup>, 440 (dec. without melting)<sup>[20]</sup>, 340 (DSC @ 20 °C/min, exo peak max.)<sup>[25]</sup>, DTA (@ 15 °C/min): 269 (nitrous and chlorous fumes)<sup>[24]</sup>, 820 (exo., peak max.)<sup>[24]</sup>, ~270 (slow thermal dec.)<sup>[62]</sup>, but begins to sublime with slow dec. @ 130 °C<sup>[65]</sup>, 420.9 (exo, DSC @ 20 °C/min, nonspherical AP)<sup>[63]</sup>, 442.2 (exo, DSC @ 20 °C/min, spherical AP)<sup>[63]</sup>, 300 (in pure state)<sup>[68]</sup>, 389 (onset, DSC)<sup>[69]</sup></p>										

	<p>Dec. occurs in three stages<sup>[18]</sup>:</p> <ul style="list-style-type: none"> <li>(i) Low <math>T</math> dec. @ 200–300 °C (@ atmospheric pressure)<sup>[18]</sup></li> <li>(ii) High <math>T</math> stage @ 350–400 °C<sup>[18]</sup></li> <li>(iii) Rapid deflagration or combustion @ ~450 °C<sup>[18]</sup></li> </ul> <p>AP dec. catalyzed by many inorganic salts<sup>[18]</sup></p> <p>Analytical-grade AP, &gt;99% purity, average particle size = 30–40 µm, TG/DSC-MS-FTIR, 2 mg sample, alumina crucible with pre-hole in lid, Ar<sup>[45]</sup>:</p> <table border="1"> <thead> <tr> <th>Heating rate (K/min)</th><th>First max. exothermic peak <math>T</math> (°C)</th><th>Second max. exothermic peak <math>T</math> (°C)</th></tr> </thead> <tbody> <tr> <td>5</td><td>302</td><td>422</td></tr> <tr> <td>10</td><td>320</td><td>434</td></tr> <tr> <td>15</td><td>330</td><td>440</td></tr> <tr> <td>20</td><td>337</td><td>441</td></tr> </tbody> </table> <p>(see additional, detailed section later)</p>			Heating rate (K/min)	First max. exothermic peak $T$ (°C)	Second max. exothermic peak $T$ (°C)	5	302	422	10	320	434	15	330	440	20	337	441
Heating rate (K/min)	First max. exothermic peak $T$ (°C)	Second max. exothermic peak $T$ (°C)																
5	302	422																
10	320	434																
15	330	440																
20	337	441																
$\rho$ [g cm <sup>-3</sup> ]	<p>1.95 (@ 298 K)<sup>[1,3,18]</sup>, 1.949<sup>[4]</sup>, 1.80, 1.95 (ortho)<sup>[12]</sup>, 1.71, 1.76 (cubic)<sup>[12]</sup>, 1.95<sup>[7,8,11,29,65,67,68]</sup>, 1.95 (@ 25 °C)<sup>[20]</sup>, 1.71 (@ 250 °C)<sup>[20]</sup>, sp. gr. = 1.95<sup>[48,68]</sup>, 1.95 (crystal, orthorhombic form)<sup>[53,59,62]</sup>, 1.76 (crystal, cubic form)<sup>[53,59]</sup>, 0.90 (nonspherical AP loading <math>\rho</math>)<sup>[63]</sup>, 1.22 (spherical AP loading <math>\rho</math>)<sup>[63]</sup></p>																	
Heat of formation	<p>−601.7 kcal/kg (enthalpy of form.)<sup>[1]</sup>, −70.6 kcal mol<sup>−1</sup><sup>[10]</sup>, 665 cal/g<sup>[7]</sup>, −70.58 kcal mol<sup>−1</sup>(<math>\Delta H_f^\circ</math>)<sup>[8]</sup>, −295 kJ mol<sup>−1</sup>(<math>\Delta H_f^\circ</math>)<sup>[8]</sup>, −70.21 kcal/mol<sup>[20]</sup>, −2,517.4 kJ/kg (enthalpy of form.)<sup>[1]</sup>, −2,518.8 kJ/kg<sup>[4]</sup>, −2,515 kJ/kg (<math>\Delta H_f^\circ</math>)<sup>[8,9]</sup>, −296 kJ mol<sup>−1</sup> (enthalpy of form.)<sup>[29,65]</sup>, −70.4 kcal mol<sup>−1</sup><sup>[18]</sup>, −70.68 kcal/mol (<math>\Delta H_f^\circ</math>, exptl.)<sup>[31]</sup>, −69.01 kcal/mol (<math>\Delta H_f^\circ</math>, calcd.)<sup>[31]</sup>, −79.7 kcal/mol (<math>\Delta H_f^\circ</math>)<sup>[34]</sup>, −295.8 kJ/mol (<math>\Delta H_f^\circ</math>)<sup>[43]</sup>, −2,517.7 J/g (<math>\Delta H_f^\circ</math>)<sup>[43]</sup>, −295.4 kJ/mol (<math>\Delta H_f^\circ</math>, exptl.)<sup>[71]</sup>, −265.7 kJ/mol (<math>\Delta H_f^\circ</math>, calcd., Born–Haber cycles)<sup>[71]</sup></p> <p><math>\Delta H_f^\circ</math> (kcal/mol) cited in<sup>[44]</sup>: 78.1 (Berthelot, 1882); 70.2 (Goodeve, 1937); 69.42 (NBS USA, 1952); 69.54 ± 0.18 (Vorob'ev, 1960); 70.63 (Birky, 1960); 69.54 ± 0.18 (Skuratov, 1961); 70.58 (NBS USA, 1965); 70.69 ± 0.30 (JANAF, 1965); 69.17 ± 0.13 (USSR, 1965); 70.58 (NBS USA, 1968); 70.69 ± 0.30 (USSR, 1971); 70.48 ± 0.12 (Kirpichev, 1973)<sup>[44]</sup>, 70.68 ± 0.09 (Matyushin)<sup>[44]</sup></p>																	
$\Delta H_c$ [kcal/mol]	$\Delta H_c = -70.7 \text{ kcal/mol}$ <sup>[50]</sup>																	
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.															

$-\Delta_{\text{ex}} U^{\circ} [\text{kJ kg}^{-1}]$	1,419	1972 [ $\text{H}_2\text{O (l)}$ @ 25 °C] (calcd. ICT code) <sup>[1,14]</sup> 1972 [ $\text{H}_2\text{O (g)}$ ] (calcd. ICT code) <sup>[43]</sup> 1970 [ $\text{H}_2\text{O (l)}$ ] <sup>[65]</sup>	1972 [ $\text{H}_2\text{O (l)}$ ] <sup>[1]</sup> 2008 <sup>[9]</sup>
$T_{\text{ex}} [\text{K}]$	1,713	780 (calcd.) <sup>[22]</sup>  1,350 °C (@ 1.00 g cm <sup>-3</sup> loading $\rho$ , calcd. based on hydrodynamic theory) <sup>[22]</sup>  1,200 °C (est.) <sup>[34]</sup>  1,084 (calcd.) <sup>[35]</sup>  2,010 (@ 1.00 g cm <sup>-3</sup> , calcd. BKWS) <sup>[10]</sup>	
$p_{\text{CJ}} [\text{kbar}]$	186	187 (calcd.) <sup>[22]</sup>  40 (@ 1.00 g cm <sup>-3</sup> , calcd. BKWS) <sup>[10]</sup>	187 (@ $\rho = 1.95 \text{ g cm}^{-3}$ ) <sup>[8]</sup>  6.32 GPa (@ 1.25 g cm <sup>-3</sup> ) <sup>[23]</sup>  9.75 GPa (@ 1.50 g cm <sup>-3</sup> ) <sup>[23]</sup>
$\text{VoD} [\text{m s}^{-1}]$	6,809	6,430 (@ 1.95 g cm <sup>-3</sup> , calcd.) <sup>[22]</sup>  3,420 (@ 1.00 g cm <sup>-3</sup> loading $\rho$ , calcd. based on hydrodynamic theory) <sup>[22]</sup>  4,020 (@ 1.00 g cm <sup>-3</sup> ; calcd. BKWS) <sup>[10]</sup>	4,390 (@ 1.950 g cm <sup>-3</sup> ) <sup>[9]</sup>  3,700 (@ 1.00 g cm <sup>-3</sup> ) <sup>[10]</sup>  2,872 mm/μs (@ 1.006 g cm <sup>-3</sup> , 2.54 cm diameter) <sup>[13]</sup>  3,258 mm/μs (@ 0.988 g cm <sup>-3</sup> , 5.08 cm diameter) <sup>[13]</sup>  3,027 mm/μs (@ 1.009 g cm <sup>-3</sup> , 3.495 cm diameter) <sup>[13]</sup>

			4,130 (@ 0.96 g cm <sup>-3</sup> ) <sup>[23]</sup> 3,400 <sup>[18]</sup> 6,450 (@ 1.95 g cm <sup>-3</sup> ) <sup>[23]</sup> 3,000 (@ 1.3 g cm <sup>-3</sup> ) <sup>[21]</sup> 4,860 (@ 1.25 g cm <sup>-3</sup> ) <sup>[23]</sup> 5,510 (@ 1.50 g cm <sup>-3</sup> ) <sup>[23]</sup> 2,500 (@ 1.17 g cm <sup>-3</sup> , Fe pipe, 35 mm diameter, Kast) <sup>[34]</sup>
$V_0$ [L kg <sup>-1</sup> ]	884	533 (calcd., ICT code) <sup>[14]</sup>  810 (est.) <sup>[34]</sup>  533 (determined for thermodynamically controlled reaction @ 25 °C without water, calcd. ICT thermodynamic code) <sup>[43]</sup>	799 <sup>[1]</sup>

Thermal behavior of AP under various conditions<sup>[38]</sup>:

- DSC (12 °C/min, open pan): 240 °C (endo, orthorhombic → cubic), 308 °C (exo), ~405 °C (endo)<sup>[38]</sup>  
 DSC (12 °C/min, sample holder with pierced lid): 240 °C (endo, orthorhombic → cubic), no endo peak, ~425 °C (exo, peak max)<sup>[38]</sup>  
 DSC (12 °C/min, ball-milled powder sample): 240 °C (endo), 279 °C (exo), ~390 °C (endo, peak max.)<sup>[38]</sup>  
 DSC (12 °C/min, grain sample): 240 °C (endo), 305 °C (exo), ~400 °C (endo, peak max.)<sup>[38]</sup>  
 DSC (12 °C/min, single crystal): 240 °C (endo), no exo, ~425 °C (endo)<sup>[38]</sup>  
 TGA (12 °C/min, ball-milled powder sample): two-step mass loss process: 279 °C (max. ~20% mass loss), ~405 °C (complete dec.)<sup>[38]</sup>  
 TGA (12 °C/min, single crystal): 1 step dec. process: 450 °C (100% mass loss)<sup>[38]</sup>  
 TGA (12 °C/min, single crystal): 1 step dec. process: ~425 °C (100% mass loss, but TGA suggests that ~12% mass is lost by the onset of the endo peak in DSC)<sup>[38]</sup>  
 TGA (12 °C/min, pellet,  $\rho = \sim 1.73$  g cm<sup>-3</sup>, from AP powder subjected to 4 ton of pressure): 275 °C (mass loss begins, 20% mass loss) ~410 (100% dec.)<sup>[38]</sup>  
 TGA (12 °C/min, pellet,  $\rho = \sim 1.85$  g cm<sup>-3</sup>, from AP powder subjected to 7 ton of pressure): 300 °C (mass loss begins, 20% mass loss) ~410 (100% dec.)<sup>[38]</sup>  
 DSC (12 °C/min, pellet, 4 ton pressure): 240 °C (endo, broadened, cf. crystals), ~320 °C (exo), ~425 °C (very broad endo peak max.)<sup>[38]</sup>  
 DSC (12 °C/min, pellet, 4 ton pressure): 240 °C (endo, broadened, cf. crystals), ~340 °C (exo), ~425 °C (very broad endo peak max.)<sup>[38]</sup>

HP-DSC (high-pressure DSC, 12 °C/min @ 0.5 MPa, single crystal): 240 °C (endo, peak max.), ~350 °C (exo, very weak), ~465 °C (peak max.)<sup>[38]</sup>  
 DSC (20 °C/min, raw AP): 246.0 (endo), 285.0 (exo), 407.9 (exo)<sup>[63]</sup>  
 DSC (20 °C/min, nonspherical AP): 246.3 (endo), 420.9 (exo)<sup>[63]</sup>  
 DSC (20 °C/min, spherical AP): 245.7 (endo), 442.2 (exo)<sup>[63]</sup>

For essentially voidless materials of ≥95% TMD, the VoD @ critical conditions ( $D_c$ ) is less than the ideal detonation velocity ( $D_i$ ), but it is only slightly less @ high % TMD<sup>[26]</sup>; however, high porosity, granular charges show much lower  $D_c/D_i$  values<sup>[26]</sup>: 25μ AP @ 51% TMD,  $D_c/D_i = 0.45^{[26]}$

Experimental test data for NG-AP composites confined in steel pipes. The addition of small quantities of NQ enabled sympathetic detonation of AP to be achieved<sup>[36]</sup>:

NQ added (wt.%)	Bulk $\rho$ (g/cc)	Pipe size (diameter) (in)	Storage >1 year?	VoD (mm/μs) <sup>†</sup>	Projectile velocity (m/s)
5	1.30	0.25	Yes	1.70	21
5	1.24	0.75	Yes	1.84	45
5	1.25	1.50	Yes	2.25	193
2.5	1.44	0.25	Yes	1.61	Lost
2.5	1.32	0.25	No	1.55	18
2.5	1.29	0.75	Yes	1.69	39
2.5	1.24	1.50	Yes	Lost	180
2.5	1.19	1.50	No	1.79	173
1..25	Caked	0.25	Yes	Failed	—
1.25	1.27	0.75	Yes	1.57	33

<sup>†</sup>Fiber optic probes in conjunction with light detectors @ six stations were used to determine the VoD.

Pipe size effect on VoD for NQ-AP composites<sup>[36]</sup>:

Pipe size	NQ (wt.%)	VoD (ideal)*	VoD (actual) (mm/μs)
0.25	5	1.70	1.70
0.75	5	1.69	1.84
1.50	5	1.69	2.25
0.25	2.5	1.58	1.61
0.25	2.5	1.57	1.55
0.75	2.5	1.57	1.69
1.50	2.5	1.56	1.79
0.75	1.25	1.50	1.57
1.50	1.25	1.50	1.69

\* Based on the equation:  $D = 4.015 \rho + 1.44$  (for NQ).

Detonation state values calculated using TIGER and three BKW parameter sets ( $D_\infty = \text{VoD} @ \text{infinite diameter}$ )<sup>[40]</sup>:

$\rho$ (g/cc)	$D_\infty$ (mm/μs)	T (K)	Parameter set
1.00	4.05	1,854	BKWR
1.95	6.49	1,497	BKWR
1.00	4.02	2,008	BKWS
1.95	6.96	1,984	BKWS
1.00	3.68	1,902	BKWC
1.95	6.42	1,772	BKWC

Calculated data from VoD- $\rho$  curves for 10 μm AP (\* is the reciprocal of the charge diameter,  ${}^{10}/_d$ )<sup>[40]</sup>:

$\rho$ (g/cc)	$D$ (mm/μs)	${}^{10}/_d ({}^{10}/_{\text{mm}})^*$	$\rho$ (g/cc)	$D$ (mm/μs)	${}^{10}/_d ({}^{10}/_{\text{mm}})^*$
0.60	~2.6	~0.0	1.10	~4.05	~0.0
0.60	~2.3	~0.13	1.10	~3.8	~0.13
0.60	~2.1	~0.2	1.10	~3.6	~0.2
0.60	~1.9	~0.29	1.10	~3.4	~0.29
0.60	~1.6	~0.39	1.10	~3.2	~0.39

Influence of the particle size on VoD of porous AP<sup>[40]</sup>:

$\rho$ (g/cc)	Particle size ( $\mu\text{m}$ )	$D$ (mm/ $\mu\text{s}$ )	$^{10}/_d$ ( $^{10}/\text{mm}$ )
1.25	6	4.4	0.1
1.25	6	~3.8	~0.16
1.00	13	~3.3	0.1
1.00	13	~3.0	~0.16
1.00	10	~3.3	0.2
1.00	10	~3.1	~0.29
1.00	10	~2.8	~0.39

Detonation sensitivity	No. 8 blasting cap is of minimum size which will detonate AP <sup>[18]</sup>											
Critical diameter [cm]	2 in (confined) <sup>[18]</sup> , 4 in (unconfined) <sup>[18]</sup> Effect of particle size ( $\delta$ ) on the critical diameter ( $d_c$ ) (critical particle size). The $d_c$ versus $\delta$ at fixed $\rho$ (1.1 g $\text{cm}^{-3}$ , 56.4% TMD) (approx. values given) <sup>[26]</sup> :											
Source of data $d_c$ (mm) $\delta$ ( $\mu\text{m}$ )      Source of data $d_c$ (mm) $\delta$ ( $\mu\text{m}$ )												
Cylindrical charge      33      50      Data for a cone      45      95												
35      50           55      120												
70      80           57      180												
65      90           72      290												
80      120           79      320												
73      125           81      580												
79      190           24      10												
70      190           39      40												
Detonability curves for different % TMDs <sup>[26]</sup> :												
Particle size, $\delta$ ( $\mu\text{m}$ )		$d_c$ (mm)	% TMD	Particle size, $\delta$ ( $\mu\text{m}$ )		$d_c$ (mm)						
10		22	30	25		38						
		21	40			55						
		22	50			40						
		25	60			60						
		36	70			70						

	Values from <sup>[47]</sup> :																																																				
	<table border="1"> <thead> <tr> <th>Material</th><th colspan="7">Critical diameter for detonation, <math>d_c</math> (mm)</th></tr> <tr> <th></th><th>70</th><th>75</th><th>80</th><th>85</th><th>90</th><th>93</th><th>98</th></tr> </thead> <tbody> <tr> <td>AP (10 µm)</td><td>29.5</td><td>47</td><td>72</td><td>&gt;76</td><td>&gt;76</td><td>&gt;76</td><td>&gt;76</td></tr> <tr> <td>AP (25 µm)</td><td>45</td><td>60</td><td>&gt;76</td><td>&gt;76</td><td>&gt;76</td><td>&gt;76</td><td>&gt;76</td></tr> </tbody> </table>	Material	Critical diameter for detonation, $d_c$ (mm)								70	75	80	85	90	93	98	AP (10 µm)	29.5	47	72	>76	>76	>76	>76	AP (25 µm)	45	60	>76	>76	>76	>76	>76																				
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Trauzl test [cm <sup>3</sup> , % TNT]	46% PA <sup>[18,21]</sup> , 220 cm <sup>3</sup> (net expansion) <sup>[34]</sup>																																																				
Sand test [g]	6 g (200 g bomb sand test) <sup>[7]</sup> , 6 g crushed by 0.4 g AP initiated by 0.25 g tetryl <sup>[18]</sup>																																																				
Ballistic mortar test	100% TNT <sup>[18]</sup> , 60% PA (ballistic mortar Mk.IIId test) <sup>[69]</sup>																																																				
Initiation efficiency	0.20 g minimum detonating charge of LA <sup>[7]</sup> , 0.25 g minimum detonating charge of tetryl <sup>[7]</sup>																																																				
LSGT [cm]	<p>Negative @ 150 cards for a slurry of AP and DMF (67% AP by weight, NOL LSGT)<sup>[52]</sup></p> <p>50% gap, all charges isostatically pressed (except <sup>a</sup> which was hydraulic pressed)<sup>[60]</sup>:</p> <table border="1"> <thead> <tr> <th>TMD (g cm<sup>-3</sup>)</th><th>Exptl. <math>\rho</math> (g cm<sup>-3</sup>)</th><th>% TMD</th><th>Gap (cards)</th></tr> </thead> <tbody> <tr> <td>1.95</td><td>1.56<sup>a</sup></td><td>80.1</td><td>87</td></tr> <tr> <td></td><td>1.57</td><td>80.6</td><td>80</td></tr> <tr> <td></td><td>1.57</td><td>80.4</td><td>71</td></tr> <tr> <td></td><td>1.58</td><td>81.1</td><td>93</td></tr> </tbody> </table>	TMD (g cm <sup>-3</sup> )	Exptl. $\rho$ (g cm <sup>-3</sup> )	% TMD	Gap (cards)	1.95	1.56 <sup>a</sup>	80.1	87		1.57	80.6	80		1.57	80.4	71		1.58	81.1	93																																
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	1.46I	75.1	113 ± 1 M	51	7	
	1.56I	80.1	80 E	63	7	
	1.56I	80.3	76 ± 2 M	65	7	
	1.57I	80.4	71 ± 1	67	7	
	1.60I	82.2	Q		7	Damage to witness plate
	1.17H	60.0	174 M	28	8	
	1.31H	67.0	171	29	8	
	1.43H	73.4	135	45	8	
	1.56H	80.1	87	62	8	
	1.25I	64.1	178E	26	11	
	1.57I	80.6	80	63	11	
	1.38I	70.7	150	36	12	
	1.52I	77.9	90 ± 2	59	12	
	0.75P	38.6	Q			Micromilled
	1.11H	56.9	198	20	25	
	1.25H	64.2	178	26	25	
	1.25H	64.4	178	26	25	
	1.49I	76.4	143	40	25	
	1.30I	76.7	143E	40	25	
	1.52I	77.7	131	45	25	
	1.58I	81.1	98 ± 1 E	56	25	
	1.58I	81.1	93	58	25	
	1.60I	81.9	98E	56	25	
	1.65I	84.4	33E	92	25	Nondetonating
	1.67I	85.5	32E	93	25	Nondetonating
	1.23P	63.0	Q		200	Nondetonating
	1.29P	66.0	133 ± 1 E	35	200	Nondetonating
	1.43H	73.2	98E	56	200	Nondetonating
	1.46H	75.0	Q		200	Nondetonating
	1.58H	80.9	74E	66	200	Nondetonating
	1.63I	83.3	Q		200	Nondetonating
	1.89I	96.7			200	Nondetonating

	C = cast, I = isostatic press, H = hydraulic press, P = packed by hand; at 0 card gap X, G and Q indicate no go, go and questionable (X = flat plate, G = hole in plate and Q = plate damage but no hole); type of test = regular unless listed as E (extended) or M (modified); all charges are conditioned and fired at 25 °C except where noted.																																				
10 s explosion T [°C]	435 <sup>[18]</sup>																																				
5 s ignition T [°C]	435 <sup>[7,22]</sup>																																				
Detonating T [°C]	436 <sup>[46]</sup> , 350 °C (deflagration point) <sup>[65]</sup>																																				
100 °C heat test [% mass loss]	0.02% mass loss in first 48 h <sup>[7]</sup> , 0.00% mass loss in second 48 h <sup>[7]</sup> , no explosions in 100 h <sup>[7]</sup> , 1% mass loss in first 48 h <sup>[18]</sup> , 1.6% = total mass lost after 96 h <sup>[18]</sup> , no explosions in 100 h <sup>[18]</sup>																																				
Thermal stability	<p>22% mass loss @ 300 °C/15 min<sup>[20]</sup>, 35% mass loss @ 300 °C/40 min<sup>[20]</sup>, 39% mass loss @ 300 °C/50 min<sup>[20]</sup>, 42.5% mass loss @ 300 °C/60 min<sup>[20]</sup></p> <p>@ 120 °C: 0 mol gas formed per mol AP in 22 h<sup>[25]</sup>, 0 mol gas formed per mol AP in 72 h<sup>[25]</sup></p> <p>@ 220 °C: 0.87 mol gas formed per mol AP in 22 h<sup>[25]</sup>, 0.9 mol gas formed per mol AP in 72 h<sup>[25]</sup></p> <p>@ 320 °C: 1.25 mol gas formed per mol AP in 22 h<sup>[25]</sup>, 1.25 mol gas formed per mol AP in 72 h<sup>[25]</sup></p> <p>TGA mass loss of AP of different particle sizes @ 225 °C<sup>[28]</sup>:</p> <table border="1"> <thead> <tr> <th colspan="2">125 µm ≤ AP ≤ 160 µm</th> <th colspan="2">AP ≥ 250 µm</th> </tr> <tr> <th>Time (min)</th> <th>m/m<sub>0</sub> (%)</th> <th>Time (min)</th> <th>m/m<sub>0</sub> (%)</th> </tr> </thead> <tbody> <tr> <td>0</td> <td>100</td> <td>0</td> <td>100</td> </tr> <tr> <td>20</td> <td>~ 100</td> <td>20</td> <td>~ 100</td> </tr> <tr> <td>40</td> <td>~ 100</td> <td>40</td> <td>~ 100</td> </tr> <tr> <td>60</td> <td>~ 92</td> <td>60</td> <td>~ 92.5</td> </tr> <tr> <td>80</td> <td>~ 80</td> <td>80</td> <td>~ 87.5</td> </tr> <tr> <td>100</td> <td>~ 73</td> <td>100</td> <td>~ 83</td> </tr> <tr> <td>120</td> <td>~ 71</td> <td>120</td> <td>~ 82.5</td> </tr> </tbody> </table>	125 µm ≤ AP ≤ 160 µm		AP ≥ 250 µm		Time (min)	m/m <sub>0</sub> (%)	Time (min)	m/m <sub>0</sub> (%)	0	100	0	100	20	~ 100	20	~ 100	40	~ 100	40	~ 100	60	~ 92	60	~ 92.5	80	~ 80	80	~ 87.5	100	~ 73	100	~ 83	120	~ 71	120	~ 82.5
125 µm ≤ AP ≤ 160 µm		AP ≥ 250 µm																																			
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80	~ 80	80	~ 87.5																																		
100	~ 73	100	~ 83																																		
120	~ 71	120	~ 82.5																																		

	Weight loss (mg) @ 211 °C vs. time <sup>[39]</sup> :					
	AP particle size (μm)	Time (min)				
		100	150	175	300	425
	3*	—	< 0.5	< 0.5	< 0.5	~ 0.5 (2%)
	25–38	—	< 0.5 (~1%)	~ 0.7 (~5%)	~ 2.3 (~15%)	~ 3.5 (~19%)
	75–106	—	~ 0.5 (~2%)	~ 1.0 (~5%)	~ 4.5 (~25%)	~ 5.0 (~28%)
	250–355	—	~ 0.5 (~5%)	~ 1.0 (~8%)	~ 6.0 (~30%)	~ 7.0 (~35%)
* No dec. occurred only sublimation. <sup>[39]</sup>						
Commercial product shows violent dec. @ 260–360 °C <sup>[65]</sup> , can dec. explosively even in the absence of fuels. <sup>[65]</sup>						
Vacuum stability test [cm <sup>3</sup> /h]	0.13 cc/40 h @ 100 °C <sup>[7]</sup> , 0.20 cc/40 h @ 120 °C <sup>[7]</sup> , 0.32 cc/40 h @ 150 °C <sup>[7]</sup>					
Vapor pressure [atm @ °C]	1.05 × 10 <sup>-8</sup> Torr @ 66 °C <sup>[19]</sup>					
Volatility	Begins @ 120 °C with all AP sublimed by 200 °C in hypodermic tube sealed at one end with the open end in mass spec. <sup>[20]</sup>					
Burn rate [mm/s]	0.33 in s <sup>-1</sup> (@ 1,000 psi for crystals) <sup>[20]</sup> , may explode in fire <sup>[48]</sup> , @ RT pure AP only burns @ $p > 20\text{--}30 \text{ atm}$ , <sup>[59]</sup> $u = 3\text{--}4 \text{ mm/s}$ @ 25 atm <sup>[59]</sup> , $u = 5\text{--}7 \text{ mm/s}$ @ 70 atm <sup>[59]</sup> , 0.16 (@ 1 atm, SMATCH/FTIR spectroscopy) <sup>[64]</sup> , 0.25 (@ 1 atm, strand burner) <sup>[64]</sup>					

Fuel	Method of preparing mixture	$\alpha$	Oxidizer particle size	$u$ (mm/s)				
				10 atm	25 atm	40 atm	75 atm	100 atm
Polystyrene (<100 $\mu\text{m}$ )	Ungelatinized*	1	Coarse Mixed Fine Y***	3.8 4.8 4.9 0.91	5.1 7.2 7.4 0.92	6.8 9.1 9.3 0.92	9.1 12.2 12.0 1.07	10.4 15.1 14.6 1.12
		0.5	Fine	5.4	7.8	10.6	14.0	16.6
	Gelatinized*	0.7	Coarse Mixed Fine Y	4.2 7.2 9.9 0.52	6.6 12.2 17.1 0.53	7.6 16.6 23.4 0.57	19.3 22.2 35.2 0.48	12.1 29.2 42.4 0.56
		0.35	Fine**	6.2	—	14.0	—	26.5
Perspex	Ungelatinized	2	Coarse Mixed Fine Y	2.7 4.9 5.4 0.82	4.4 7.9 10.6 11.1	5.3 10.6 10.7 14.5	7.5 12.9 10.7 0.98	8.0 15.8 16.2 0.95
		1	Fine	7.0	—	—	—	22.8
	Ungelatinized	1	Coarse Mixed Fine Y	3.2 4.0 5.7 0.32	4.7 5.3 8.1 0.18	5.2 5.8 9.1 0.15	7.0 7.3 12.7 0.9	7.5 16.2 0.95 0.9
		0.5	Fine	3.3	4.2	3.9	4.0	6.0
Perspex (~3 $\mu$ )	Ungelatinized	0.7	Coarse Mixed Fine Y	3.5 4.0 4.5 0.50	4.8 5.2 5.4 0.67	5.7 5.6 6.2 —0.2	8.2 7.4 7.8 —1.6	8.2 7.4 8.7 —1.6
		0.35	Fine	—	Does not burn	—	—	—

\*The ungelatinized mixture was prepared by mixing the components in powder form. The gelatinized mixture was prepared in the same way, then treated with solvent (dichloroethane), mixed for 24 h and dried. During gelatinization, the fuel was spread as a film over the surface of the oxidizer particles. \*\*Data obtained by interpolation on curve  $u(d)$ . \*\*\*Y =  $u_{\text{mixed}} - u_{\text{coarse}} / |u_{\text{fine}} - u_{\text{coarse}}|$

Burning rate of compositions based on  $\text{NH}_4\text{ClO}_4$  with fine ( $\sim 5 \mu\text{m}$ ), coarse ( $140\text{--}320 \mu\text{m}$ ) and mixed (50% fine + 50% coarse) oxidizer, data from<sup>[59]</sup>:

Influence of pressure on efficacy of catalysts on burning rate of pure  $\text{NH}_4\text{ClO}_4$  (numerical data taken from graphs; \*  $Z = u_{\text{with catalyst}}/u_{\text{without catalyst}}$ )<sup>[59]</sup>:

Catalyst	Pressure (atm)							
		50	60	70	80	90	100	150
No catalyst	$u$ (mm/s)	6.3	7.2	8.2	8.9	9.5	10.2	12.3
3% copper chromite	$u$ (mm/s)	11.1	17.1	23.2	27.4	30.7	33.6	43.6
	$Z^*$	1.76	2.36	2.83	3.08	3.23	3.30	3.55
5% copper chromite	$u$ (mm/s)	22.2	26.1	30	32.8	35.2	38	46.8
	$Z^*$	3.52	3.60	3.66	3.68	3.71	3.73	3.81

Effect of particle size of AP powder from which charges are pressed ( $\delta \approx 1$ ) on the burning rate,  $\mu$  = particle size, <sup>†</sup> @ 105 atm pressure and <sup>‡</sup> @ 100 atm<sup>[59]</sup>:

Fraction $\text{NH}_4\text{ClO}_4$ ( $\mu\text{m}$ )	$u$ (mm/s)	Coating material	Diameter of charge (mm)	
~ 15	12	Cement + glass	10	†
< 100	9.9	Cement + glass	10	†
100–140	10	Cement + glass	10	†
~ 15	11.4	Perspex	6	†
320–410	12	Perspex	6	†
53–66	8.9	Uncoated	5 × 5	‡
66–76	8.6	Uncoated	5 × 5	‡
76–104	7.9	Uncoated	5 × 5	‡

Mean values of the burning rate can be used for tentative comparisons, pure AP, data from<sup>[59]</sup>:

$p$ (atm)	40	60	80	100
$\bar{u}$ (mm/s)	4	6	8	10

	Dependence of $u(\delta)$ for AP (particle size 100–140 $\mu\text{m}$ ) in an inert casing (for $\delta \approx 1$ phosphate cement-glass; for $\delta = 0.75$ and 0.65, glass; diameter of charge = 10 mm) <sup>[59]</sup> :						
$p$ (atm)	$u$ (mm/s)			$u\delta$			
	$\delta = 1$	$\delta = 0.75$	$\delta = 0.65$	$\delta = 1$	$\delta = 0.75$	$\delta = 0.65$	
60	6.6	4.6	—	6.6	3.4	—	
100	10.0	6.7	6.5	10.6	5.0	4.2	
	Dependence of $u(\delta)$ for $\text{NH}_4\text{ClO}_4$ in a perspex casing (diameter of charge = 6 mm):						
$\text{NH}_4\text{ClO}_4$ particle size ( $\mu\text{m}$ )	$p$ (atm)	$u$ (mm/s)			$u\delta$		
		$\delta = 0.96$	$\delta = 0.72$		$\delta = 0.96$	$\delta = 0.72$	
15	5	0.68	1.0		0.65	0.72	
	10	1.5	1.6		1.44	1.15	
	40	4.9	5.9		4.7	4.25	
	100	11.4	12.6		11.0	9.1	
320–410	5	0.63	0.78		0.6	0.56	
	10	1.04	1.55		1.0	1.1	
	40	5.4	Sudden change in burning rate		5.2	—	
	100	12.0	Sudden change in burning rate		11.5	—	
	$\text{NH}_4\text{ClO}_4$ ( $\approx 15 \mu\text{m}$ ) with the addition of 2% $\text{Cu}_2\text{O}$ ( $p = 1$ atm abs., glass casing, $\phi = 10$ mm): <sup>[59]</sup>						
$\delta$		0.84	0.62	0.59	0.54	0.38	
$u\delta$ (mm/s)		0.92	0.98	0.94	0.94	0.95	
	Dependence of $u(\delta)$ for pure $\text{NH}_4\text{ClO}_4$ with an inert casing at an elevated initial temperatre (pressure 20 atm); @ 150 °C the mass burning rate is almost independent of $\delta$ : <sup>[59]</sup>						
$\delta$		$u\delta$ (mm/s)	$T_0$ (°C)	$\delta$	$u\delta$ (mm/s)	$T_0$ (°C)	
0.98		3.3	100	0.98	4.4	150	
0.75		2.9	100	0.62	4.2	150	
0.62		2.5	100				

Flame $T$	<p>Calcd. flame <math>T</math> as monopropellant and as a component of stoichiometric mixtures with a high-grade paraffin as fuel <math>[(\text{CH}_2)_n]</math> with <math>\Delta H_f = -5.971 \text{ kcal/mol}</math> @ 298 K<sup>[20]</sup>:</p> <table border="1" data-bbox="393 255 991 388"> <thead> <tr> <th colspan="2">Monopropellant combustion</th><th colspan="2">Stoichiometric combustion</th></tr> <tr> <th><math>T(\text{K}), 1 \text{ atm}</math></th><th><math>T(\text{K}), 1,000 \text{ psi}</math></th><th><math>T(\text{K}), 1,000 \text{ psi}</math></th><th>S.I. (lb s/lb)</th></tr> </thead> <tbody> <tr> <td>1,390</td><td>1,417</td><td>2,997</td><td>252.0</td></tr> </tbody> </table> <p>Ammonia and perchloric acid vapor burn near the crystal surface with calcd. flame <math>T</math> of 1,380 K @ 1 atm<sup>[59]</sup></p>	Monopropellant combustion		Stoichiometric combustion		$T(\text{K}), 1 \text{ atm}$	$T(\text{K}), 1,000 \text{ psi}$	$T(\text{K}), 1,000 \text{ psi}$	S.I. (lb s/lb)	1,390	1,417	2,997	252.0		
Monopropellant combustion		Stoichiometric combustion													
$T(\text{K}), 1 \text{ atm}$	$T(\text{K}), 1,000 \text{ psi}$	$T(\text{K}), 1,000 \text{ psi}$	S.I. (lb s/lb)												
1,390	1,417	2,997	252.0												
Solubility [g/mL]	<p>12 g/100 cc in <math>\text{H}_2\text{O}</math> @ 0 °C<sup>[7]</sup>, 20 g/100 cc in <math>\text{H}_2\text{O}</math> @ 25 °C<sup>[7]</sup>, 39 g/100 cc in <math>\text{H}_2\text{O}</math> @ 60 °C<sup>[7]</sup></p> <p>Aqueous solubility g/100 g <math>\text{H}_2\text{O}</math><sup>[27]</sup>:</p> <table border="1" data-bbox="393 631 730 940"> <thead> <tr> <th><math>T(\text{°C})</math></th><th>Solubility (g/100 g <math>\text{H}_2\text{O}</math>)</th></tr> </thead> <tbody> <tr> <td>0</td><td>~10</td></tr> <tr> <td>10</td><td>~15</td></tr> <tr> <td>20</td><td>~25</td></tr> <tr> <td>30</td><td>~30</td></tr> <tr> <td>40</td><td>~35</td></tr> <tr> <td>60</td><td>~50</td></tr> </tbody> </table> <p>12.4 parts AP per 100 parts <math>\text{H}_2\text{O}</math> @ 0 °C<sup>[35]</sup>, 88.2 parts AP per 100 parts <math>\text{H}_2\text{O}</math> @ 100 °C<sup>[35]</sup>, soluble in <math>\text{H}_2\text{O}</math><sup>[46,48]</sup>, slightly soluble in EtOH and acetone<sup>[46]</sup>, insoluble in <math>\text{Et}_2\text{O}</math><sup>[46]</sup>, 6.85 g/100 g MeOH<sup>[20]</sup>, 1.91 g/100 g EtOH<sup>[20]</sup>, 0.39 g/100 g <i>n</i>-propanol<sup>[20]</sup>, 0.017 g/100 g <i>n</i>-butanol<sup>[20]</sup>, 2.26 g/100 g acetone<sup>[20]</sup>, insoluble in <math>\text{Et}_2\text{O}</math><sup>[20]</sup>, 20 g/L water @ 15 °C<sup>[62]</sup>, slightly soluble in acetone and EtOH<sup>[62]</sup>, 24 g/100 g <math>\text{H}_2\text{O}</math> @ 25 °C<sup>[65]</sup>, freely soluble in water<sup>[67]</sup>, soluble in MeOH<sup>[67]</sup>, slightly soluble in EtOH, acetone<sup>[67]</sup>, almost insoluble in ethyl acetate, <math>\text{Et}_2\text{O}</math>.<sup>[67]</sup></p> <p>Solubility in DMF after 5 min stirring<sup>[52]</sup>: 46 g/100 g DMF @ 0 °C<sup>[52]</sup>, 47 g/100 g DMF @ 25 °C<sup>[52]</sup></p>	$T(\text{°C})$	Solubility (g/100 g $\text{H}_2\text{O}$ )	0	~10	10	~15	20	~25	30	~30	40	~35	60	~50
$T(\text{°C})$	Solubility (g/100 g $\text{H}_2\text{O}$ )														
0	~10														
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30	~30														
40	~35														
60	~50														
Hygroscopicity	<p>Deliquescence of ultra-fine AP strikingly deteriorated with decreasing particle size<sup>[33]</sup>, ultra-fine AP shows <math>\text{H}_2\text{O}</math> absorption under the atmosphere of saturated steam, and the hygroscopicity increases sharply to ~12% &gt; 400 °C<sup>[33]</sup>, nonhygroscopic<sup>[46]</sup>, critical humidity = 95.6% RH @ 15 °C<sup>[66]</sup></p>														

	Hygroscopicity of ultra-fine AP <sup>[33]</sup> :			
	Time (h)	Hygroscopicity (%)	Time (h)	Hygroscopicity (%)
	25	~2	200	~7.5
	50	~2.5	275	~9.5
	75	~3	330	~10.5
	90	~3.5	355	~11
	140	~5.5	425	~12
Photosensitivity	No photolysis expected <sup>[51]</sup>			
Compatibility	AP dec. catalyzed by many inorganic salts <sup>[18]</sup>  Effect of various additives on thermal dec. of NH <sub>4</sub> ClO <sub>4</sub> <sup>[20]</sup> :			
	Additive	Observed effect		
	NH <sub>3</sub> gas	Dec. stopped at any temperature up to 400 °C		
	HCl gas	Accelerated the dec. to 30% – no further effect. No effect on induction period		
	Cl <sub>2</sub> gas	Accelerated the dec. to 30%, which then continued to completion. No effect on induction period		
	KClO <sub>3</sub>	Accelerated dec. to 30%, then dec. at normal rate. Induction period reduced but not eliminated, log τ versus $1/\tau$ gave 25.5 kcal/mol. No increase in burning rate @ 300–2,500 psi		
	Copper chromite	DTA results in deflagration @ 320 °C. Under ammonia, detonation occurs @ the same T. Isothermal study @ 265 °C resulted in detonation		
	Pressure	DTA shows exotherm @ 310 °C. As pressure increases, so does the rate of dec.		
	(NH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub> (NH <sub>4</sub> ) <sub>2</sub> C <sub>2</sub> O <sub>4</sub>	$T$ of first exotherm in DTA increases from ~310 °C to ~400 °C		

Catalyzed decomposition of AP data from [20]:

	<p>Equation (1), <math>\log[\alpha/1 - \alpha] = kt + C</math>: acceleratory; eq. (2), <math>\log[\alpha/1 - \alpha] = kt + C</math>: decelerator; eq. (3), <math>\log p = kt + C</math>; eq. (4), <math>\log \omega = kt + C</math>; <math>(\log(1/1 - \alpha)) = kt + C</math>; eq. (5), <math>\log \tau = E/RT + C</math>; <math>\tau</math> is time to ignition (initiation); eq. (6), <math>[-\log(1 - \alpha)]^{1/3} = kt</math>: Avrami-Erofeev, <math>n = 3</math>; eq. (7), <math>\log(dT/dt) = -E/RT + C</math>: adiabatic kinetics</p> <p>Decomposition of AP with cocrystallized or mechanically mixed catalysts (CC = cocrystallized; MM = mechanically mixed)<sup>[20]</sup>:</p>																																																			
	<table border="1"> <thead> <tr> <th>Sample</th><th>Catalyst type*</th><th>T (°C)</th><th>Heating time (min)</th><th>Wt. loss (%)</th></tr> </thead> <tbody> <tr> <td>AP + 2% CaCrO<sub>4</sub></td><td>CC</td><td>233</td><td>4</td><td>88</td></tr> <tr> <td>AP + 2% CaCrO<sub>4</sub></td><td>MM</td><td>233</td><td>60</td><td>17.5</td></tr> <tr> <td rowspan="4">AP + 2% TiClO<sub>4</sub></td><td rowspan="4">CC</td><td>300</td><td>15</td><td>36</td></tr> <tr> <td>300</td><td>40</td><td>50</td></tr> <tr> <td>300</td><td>50</td><td>54.5</td></tr> <tr> <td>300</td><td>60</td><td>58.5</td></tr> <tr> <td rowspan="5">AP pure</td><td rowspan="5">-</td><td>300</td><td>15</td><td>22</td></tr> <tr> <td>300</td><td>40</td><td>35</td></tr> <tr> <td>300</td><td>50</td><td>39</td></tr> <tr> <td>300</td><td>60</td><td>42.5</td></tr> <tr> <td>176</td><td>20</td><td>99</td></tr> <tr> <td></td><td>MM</td><td>208</td><td>60</td><td>8</td></tr> </tbody> </table>	Sample	Catalyst type*	T (°C)	Heating time (min)	Wt. loss (%)	AP + 2% CaCrO <sub>4</sub>	CC	233	4	88	AP + 2% CaCrO <sub>4</sub>	MM	233	60	17.5	AP + 2% TiClO <sub>4</sub>	CC	300	15	36	300	40	50	300	50	54.5	300	60	58.5	AP pure	-	300	15	22	300	40	35	300	50	39	300	60	42.5	176	20	99		MM	208	60	8
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	<p>Thermal dec. is catalyzed by compounds of iron, chromium and copper and copper chromite in particular<sup>[62]</sup>, incompatible in contact or as mixtures with chlorates due to possible formation of spontaneously explosive ammonium chlorate<sup>[65]</sup>, KNO<sub>3</sub> should not be applied directly to composition containing AP<sup>[65]</sup>, reacts with Mg in the presence of moisture which can result in spontaneous ignition<sup>[65]</sup>, forms impact-sensitive mixtures with many fuels such as red phosphorus, sulfur, Sb<sub>2</sub>S<sub>3</sub>, arsenic sulfides<sup>[65]</sup>, not to be stored with reducing agents, organic materials (in particular, fuels, oils, greases)<sup>[68]</sup></p>																																																			
$\Delta H^\circ_{\text{sol}}$ [kcal/mol]	$8.060 \pm 0.006$ (measured, 99.98 ± 0.02% purity) <sup>[44]</sup>																																																			
Activation energy to decomposition [kJ/mol]	52 (first step dec.) <sup>[45]</sup> , 142 (second step dec.) <sup>[45]</sup> , 218 (third step dec.) <sup>[45]</sup>																																																			
$\Delta H_{\text{phase transition}}$ [kcal/mol]	$2.3 \pm 0.2$ <sup>[53]</sup> , 2.7 <sup>[53]</sup> , -2.3 kcal/mol (orthorhombic → cubic) <sup>[59]</sup>																																																			
Log $K_{\text{ow}}$	-5.85 (predicted) <sup>[51]</sup>																																																			

$K_{oc}$	96.6 (predicted) <sup>[51]</sup>
Koenen test	Critical diameter = 3.0 mm, result = violent <sup>[69]</sup>
Dutch pressure vessel test	Critical diameter = 6.0 mm <sup>[69]</sup>
Thermal explosion vessel test	Max. rate × max. pressure $\geq$ 403 MPa <sup>2</sup> /s, result = violent <sup>[69]</sup>
Detonability	BAM 50/60 tube test (detonator + 50 g RDX): fragmented length = 50 cm, result = detonation <sup>[69]</sup> , BAM 50/60 tube test (detonator only): fragmented length = 0 cm <sup>[69]</sup>
High-pressure autoclave test	$F$ -value = partial reaction <sup>[69]</sup>
UN princess incendiary spark test	Failed to ignite <sup>[69]</sup>
Flashpoint [°C]	310 <sup>[70]</sup>

[1] R. Meyer, J. Köhler, A. Homburg, *Explosives*, 7th edn., Wiley-VCH, Weinheim, 2016, pp. 15–16.

[2] P. A. Koutentis, *Molecules*, 2005, 10, 346–359.

	$\text{AP}^{[8,15,16]}$	$\text{AP}^{[17]}$	$\text{AP}^{[17]}$	$\text{AP}^{[17]}$	$\text{AP}^{[53,56]}$	$\text{AP}^{[54]}$	$\text{AP}^{[55]}$	$\text{AP}^{[53,57]}$
Phase <240 °C	Phase >240 °C							
Chemical formula	$\text{H}_4\text{NO}_4\text{Cl}$							
Molecular weight [g mol <sup>-1</sup> ]	117.49	117.49	117.49	117.49	117.49	117.49	117.49	117.49
Crystal system	Orthorhombic	Cubic	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic	Cubic
Space group	$P\ n\ a\ 2_1$ (no. 33)	$F\bar{4}3\ m$	$Pnma$ (no. 62)	$F\bar{4}3\ m$ (no. 216)				
$a$ [Å]	9.220(1)	7.67	9.226	9.23	9.202	9.13	9.2	7.63
$b$ [Å]	7.458(1)	7.67	5.817	7.45	5.816	5.79	5.82	7.63
$c$ [Å]	5.814(1)	7.67	7.459	5.82	7.449	7.47	7.45	7.63
$\alpha$ [°]	90	90	90	90	90	90	90	90
$\beta$ [°]	90	90	90	90	90	90	90	90
$\gamma$ [°]	90	90	90	90	90	90	90	90
$V$ [Å <sup>3</sup> ]	399.7903		400.307	400.204		398.9	444.2	
$Z$	4		4	4		4	4	
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.71		1.94944	1.94995		1.952		
$T$ [K]			<240 °C	<240 °C	RT			

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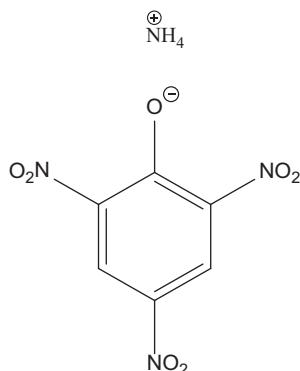
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## Ammonium picrate

Name [German, acronym]: Ammonium picrate, ammonium-2,4,6-trinitrophenolate, explosive D, dunnite, ammonium 2,4,6-trinitrophenoxide, picric acid ammonium salt, ammonium carbazoate, ammonium picronitrate, 2,4,6-trinitrophenol ammonium salt [ammonpikrat, ammoniumpikrat]

Main (potential) use: Explosive in military charges<sup>[1]</sup>, in World War I and World War II in armor-piercing shells<sup>[27]</sup>, main-charge explosive which is used in explosive ordnance which must be able to withstand severe shock and stress before detonating, for example, armor-piercing bombs, projectiles<sup>[36]</sup>, standard main charge for navy projectiles >3 in caliber<sup>[36]</sup>, bursting charge for armor-piercing projectiles<sup>[37]</sup>, ingredient of picratol<sup>[37]</sup>, standard bursting charge for armor-piercing shells<sup>[38,40]</sup>, armor-piercing projectiles<sup>[17]</sup>, jet-assisted take-off units for aircraft<sup>[17]</sup>, organic fuel in composite propellants<sup>[40]</sup>, armor piercing and demolition shells<sup>[43]</sup>, in colored flame and whistle compositions<sup>[48]</sup>, explosives, fireworks, rocket propellants<sup>[50]</sup>

Structural formula:



	Explosive D
Formula	C <sub>6</sub> H <sub>6</sub> N <sub>4</sub> O <sub>7</sub>
Molecular mass [g mol <sup>-1</sup> ]	246.14

Appearance at RT	Yellow monoclinic crystals (stable form) <sup>[17]</sup> and as red orthorhombic crystals (metastable form) <sup>[17]</sup> , yellow-orange solid (product manufactured for military use) <sup>[17]</sup> , two forms: (i) yellow crystals (solid, stable form) and (ii) red crystals (solid, metastable form) <sup>[27,28]</sup> , color is due to pH of soln. in which ammonium picrate was neutralized; red favored by higher pH <sup>[27]</sup> , crystalline material is either yellow, yellow-orange or red <sup>[36]</sup> , yellow-orange crystalline solid <sup>[37]</sup> , yellow-red crystals or granules <sup>[38]</sup> , yellow-orange solid <sup>[40]</sup> , yellow or red crystals (different modifications) <sup>[43]</sup> , bright red when freshly prepared which slowly changes to yellow form when in contact with water for several months <sup>[48]</sup> , bright yellow bitter scales or orthorhombic crystals <sup>[50]</sup> , “red modification” is not a distinct polymorph but is instead a slightly contaminated form of the yellow salt <sup>[50]</sup> , fine golden crystals <sup>[53]</sup>						
IS [J]	<p>33<sup>[2]</sup>, 8.47 (17 in, 2 kg mass, 18 mg sample, P.A.)<sup>[11]</sup>, 33.35<sup>[12]</sup>, 16–17 in (2 kg mass, P.A.)<sup>[16]</sup>, &gt;100 cm (2 kg mass, B.M.)<sup>[18]</sup>, 50% point = 254 cm (NOL-ERL apparatus)<sup>[19]</sup>, 10% explosions from 10 kg mass falling ~ 20 cm<sup>[27]</sup>, 108 cm (NEDED)<sup>[31]</sup>, 235 cm (NOL)<sup>[31]</sup>, 136 cm (LANL)<sup>[31]</sup>, <math>H_{50}</math> = 110 cm (Bruceton method, NOL machine, type 12 tool, 2.5 kg mass, 35 ± 2 mg sample, 5/0 sandpaper)<sup>[34]</sup>, <math>H_{50}</math> = 135 cm (2.5 kg mass, type 12 tool)<sup>[35]</sup>, 28 in (2 kg mass, confined, height of no detonation, P.A.)<sup>[39]</sup>, 17 in (2 kg mass, P.A.)<sup>[40]</sup>, 100 cm (2 kg mass)<sup>[43]</sup>, 17 in (18 mg sample, P.A.)<sup>[44]</sup>, 100 + cm (B.M.)<sup>[44]</sup>, 43.2 cm (P.A.)<sup>[51]</sup>, &gt;100 cm (B.M.)<sup>[51]</sup></p> <p>Powdered samples: <math>H_{50\%}</math> = 254 cm (NOL)<sup>[18]</sup>, <math>H_{50\%}</math> = 190 cm (LASL)<sup>[18]</sup>, <math>H_{50\%}</math> = 17 in (P.A.)<sup>[18]</sup></p> <p>80 cm (ERL #3, sample in brass cup 0.308 in inside diameter, 0.01 in thick, <math>\frac{7}{8}</math> in height, 5 kg mass)<sup>[55]</sup>, 19 cm (ERL #5, sample in cylindrical cavity <math>\frac{1}{16}</math> in deep, 0.376 in inside diameter, 5 kg mass)<sup>[55]</sup>, 235 cm (ERL #12, sample on square of Flint paper, <math>2\frac{1}{2}</math> kg mass)<sup>[55]</sup>, <math>H_{50\%}</math> = 59 cm (4 kg mass, B.M. design 5)<sup>[55]</sup>, <math>H_{50\%}</math> = 75 cm (5 kg mass, plane sandblasted surfaces)<sup>[55]</sup>, 100 cm (sensitivity to glancing impact, Hercules sliding rod, sandblasted surfaces, 45° slide angle, 10 lb rod, 30 mg sample)<sup>[55]</sup></p> <p>IS data from<sup>[57]</sup>:</p> <table border="1"> <thead> <tr> <th>Type 12, <math>H_{50}</math> (cm)</th> <th>Type 12B, <math>H_{50}</math> (cm)</th> </tr> </thead> <tbody> <tr> <td>136 ± 0.05</td> <td>220 ± 0.05</td> </tr> <tr> <td>137 to &gt;320</td> <td>220 to &gt;320</td> </tr> </tbody> </table> <p><math>H_{50}</math> = 79 cm (design no. 3 apparatus, 5 kg hammer)<sup>[58]</sup>, <math>H_{50}</math> = 80 cm (design no. 3 apparatus)<sup>[58]</sup>, <math>H_{50}</math> = 19 cm (design no. 5 apparatus)<sup>[58]</sup>, <math>H_{50}</math> (average) = 286 cm (design no. 7 apparatus, 5 kg hammer)<sup>[58]</sup>, <math>H_{50}</math> (average) = 264 cm (design no. 7 apparatus, 2.5 kg hammer, 1 ply tin foil)<sup>[58]</sup>, <math>H_{50}</math> (average) = 107 cm (design no. 8 apparatus, 5 kg mass)<sup>[58]</sup>, <math>H_{50}</math> (average) = 211 cm (design no. 8 apparatus, 2.5 kg hammer)<sup>[58]</sup>, <math>H_{50}</math> (average) = 308 cm (design no. 9 apparatus, 2.5 kg hammer)<sup>[58]</sup>, <math>H_{50} \leq 100</math> cm (design no. 10 apparatus, 2.5 kg hammer, tin foil covering)<sup>[58]</sup>, <math>H_{50}</math> = 99 cm (design no. 11 apparatus, 2.5 kg hammer)<sup>[58]</sup>, <math>H_{50}</math> = 87 cm (design no. 12 apparatus, 116 units, cf. TNT = 100 units)<sup>[58]</sup></p>	Type 12, $H_{50}$ (cm)	Type 12B, $H_{50}$ (cm)	136 ± 0.05	220 ± 0.05	137 to >320	220 to >320
Type 12, $H_{50}$ (cm)	Type 12B, $H_{50}$ (cm)						
136 ± 0.05	220 ± 0.05						
137 to >320	220 to >320						

FS [N]	Unaffected by steel shoe (friction pendulum test) <sup>[11,16]</sup> , unaffected by fiber shoe (friction pendulum test) <sup>[11,17,44]</sup> , unaffected in Picatinny Arsenal friction test <sup>[51]</sup> , pendulum friction test: passed fiber shoe <sup>[52]</sup> , pendulum friction test: passed steel shoe <sup>[52]</sup>																														
ESD [J]	<p><math>0.76 \pm 0.08^{[3]}</math>, 6.0 (confined, 100 mesh)<sup>[11,17]</sup>, 0.025 (unconfined, 100 mesh)<sup>[11,17]</sup>, <math>E_{50\%} = 0.76 \pm 0.08</math> (Bruceton method)<sup>[30]</sup>, 0.025 (unconfined, B.M.)<sup>[44]</sup>, 6.0 (confined, B.M.)<sup>[44]</sup></p> <p>Highest electrostatic discharge energy @ 5,000 V for zero ignition probability<sup>[22]</sup>:</p> <table border="1"> <thead> <tr> <th>Sample</th> <th colspan="2">Highest energy (J) for Zero ignition probability</th> <th colspan="2">Type of ignition</th> </tr> <tr> <th></th> <th>Unconfined</th> <th>Confined</th> <th>Unconfined</th> <th>Confined</th> </tr> </thead> <tbody> <tr> <td>Ammonium picrate (bulk)</td> <td>&gt;12.5</td> <td>6.0</td> <td>None</td> <td>Detonation</td> </tr> <tr> <td>Ammonium picrate (through 100 mesh)</td> <td>0.025</td> <td>6.0</td> <td>Deflagration</td> <td>Detonation</td> </tr> </tbody> </table> <p>0.400 (40,000 V, for zero ignition, 500 MMF capacitance, 0.005 in gap setting)<sup>[49]</sup></p> <p>Highest energy (J) for zero ignition probability<sup>[49]</sup>:</p> <table border="1"> <thead> <tr> <th>Explosive</th> <th>Determined data<sup>[49]</sup></th> <th>Bureau of Mines, 1943</th> <th>Bureau of Mines, 1946</th> <th>Bureau of Mines, 1954</th> </tr> </thead> <tbody> <tr> <td>Explosive D</td> <td>0.400</td> <td>0.10</td> <td>0.025</td> <td>0.16</td> </tr> </tbody> </table> <p>0.025 (static electricity, unconfined)<sup>[51]</sup>, 6.0 (static electricity, confined)<sup>[51]</sup></p>	Sample	Highest energy (J) for Zero ignition probability		Type of ignition			Unconfined	Confined	Unconfined	Confined	Ammonium picrate (bulk)	>12.5	6.0	None	Detonation	Ammonium picrate (through 100 mesh)	0.025	6.0	Deflagration	Detonation	Explosive	Determined data <sup>[49]</sup>	Bureau of Mines, 1943	Bureau of Mines, 1946	Bureau of Mines, 1954	Explosive D	0.400	0.10	0.025	0.16
Sample	Highest energy (J) for Zero ignition probability		Type of ignition																												
	Unconfined	Confined	Unconfined	Confined																											
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Explosive	Determined data <sup>[49]</sup>	Bureau of Mines, 1943	Bureau of Mines, 1946	Bureau of Mines, 1954																											
Explosive D	0.400	0.10	0.025	0.16																											
N [%]	22.76																														
$\Omega(\text{CO}_2)$ [%]	-52.0																														
$T_{\text{phase transition}}$ [°C]	Yellow monoclinic crystals are the stable form and red rhombic crystals are the metastable form, and the two forms are interconvertible <sup>[37]</sup> , red form is obtained when freshly prepared but slowly changes on contact with water for several months to yellow form <sup>[48]</sup> , red form is a metastable crystalline form <sup>[48]</sup> , “red modification” is not a distinct polymorph but is instead a slightly contaminated form of the yellow salt <sup>[50]</sup>																														
$T_{\text{m.p.}}$ [°C]	265–271 <sup>[4]</sup> , 265 (dec.) <sup>[11, 36, 44]</sup> , ~280 (with dec.) <sup>[12,17]</sup> , 265–270 (fusing) <sup>[43]</sup> , 265–271 <sup>[4]</sup> , ~280 (with dec.) <sup>[12,17]</sup> , <265 (dec. without melting) <sup>[16]</sup> , 265–271 (with dec.) <sup>[28]</sup> , 265–270 <sup>[37]</sup> , does not melt on heating but explodes when heated to 300 °C <sup>[38]</sup> , does not melt <sup>[40]</sup>																														
$T_{\text{dec.}}$ [°C]	>265 (dec. without melting) <sup>[11,16]</sup> , 265 <sup>[18]</sup> , 300 (explodes) <sup>[18]</sup> , 220 <sup>[43]</sup> , 265–271 <sup>[48]</sup>																														

$\rho$ [g cm <sup>-3</sup> ]	1.72 <sup>[5,47,48,50,57]</sup> , 1.717 (@ TMD) <sup>[12]</sup> , sp. gr. = 1.72 <sup>[43]</sup> , 1.717 (crystal) <sup>[16,17]</sup> , 1.72 (crystal) <sup>[11,18,44]</sup> , 1.63 (nominal) <sup>[17]</sup> , 1.719 (crystal) <sup>[37]</sup> , 1.55 (p) <sup>[55]</sup>	
Loading $\rho$ at different pressures:		
Loading $\rho$ (g/cm <sup>3</sup> )	Pressure ( $\times 10^3$ psi)	
1.33	3 <sup>[11,17,44]</sup>	
1.41	5 <sup>[11,17,44]</sup>	
1.47	10 <sup>[11,17,44]</sup>	
1.49	12 <sup>[11,17,44]</sup>	
1.51	15 <sup>[11,17]</sup>	
1.53	20 <sup>[11,17]</sup>	
1.59	50 <sup>[17]</sup>	
1.64	100 <sup>[17]</sup>	
1.61 @ 15,000 psi <sup>[44]</sup> , 1.64 @ 20,000 psi <sup>[44]</sup>		
Loading $\rho$ at different pressures: <sup>[18]</sup>		
Loading $\rho$ (g/cm <sup>3</sup> )	Pressure (kpsi)	
1.33	3	
1.41	5	
1.47	10	
1.49	12	
1.61	15	
1.64	20	
1.72	Crystal	
$\rho$ of red and yellow forms at different pressure <sup>[27]</sup> :		
Pressure (kg/cm <sup>2</sup> )	$\rho$ (g/cm <sup>3</sup> )	
	Yellow form	Red form
0 (loose)	0.891	1.045
110	1.244	1.299
330	1.396	1.392
660	1.490	1.490
1,100	1.553	1.529
1,540	1.593	1.562
1,910	1.596	1.569
2,540	1.616	1.582

Heat of formation	<p>-375.4 kcal/kg (enthalpy of form.)<sup>[1]</sup>, 395 cal/g<sup>[11,16,20]</sup>, -393 kJ/mol (<math>\Delta H_f</math>)<sup>[12]</sup>, -94.0 kcal mol<sup>-1</sup><sup>[13]</sup>, -1,570.7 kJ/kg<sup>-1</sup> (enthalpy of form.)<sup>[1]</sup>, 95.82 kg cal/mol<sup>[16,17]</sup>, -83.7 kcal/mol (<math>\Delta H_f</math>, yellow form)<sup>[27]</sup>, -93.7 kcal/mol (<math>\Delta H_f</math>, red form)<sup>[27]</sup>, 395 cal/g<sup>[11]</sup>, 354.8 kcal/kg<sup>[42]</sup>, -90.16 kcal/mol (<math>\Delta H_f^\circ</math>, exptl.)<sup>[33]</sup>, -90.18 kcal/mol (<math>\Delta H_f^\circ</math>, calcd.)<sup>[33]</sup>, -393 kJ/mol (<math>\Delta H_f</math>)<sup>[47]</sup>, -386.4 kJ/mol (enthalpy of form., exptl.)<sup>[54]</sup>, -394.7 kJ/mol (enthalpy of form., calcd., emp.)<sup>[54]</sup>, 97.04 kcal/mol (-<math>\Delta H_f</math>, heat of form. @ standard conditions)<sup>[56]</sup></p>																			
Heat of combustion [kJ mol <sup>-1</sup> ]	<p>2,745 cal/g (<math>Q_c^P</math>)<sup>[16,17]</sup>, 2,890 cal/g (<math>Q_c^V</math>)<sup>[11,16]</sup>, 685 kcal/mol (<math>Q_c^V</math>)<sup>[16]</sup>, 2,890 kcal/kg<sup>[20,44]</sup>, 687.3 kcal mol<sup>-1</sup> (red form)<sup>[27]</sup>, 677.3 kcal mol<sup>-1</sup> (yellow form)<sup>[27]</sup>, 2,760 kcal/kg @ C<sup>[42]</sup>, heat of comb. = 674.76 kcal/mol (@ 1 atm)<sup>[55]</sup></p> <p>Exptl. heat of combustion data<sup>[56]</sup>:</p> <table border="1"> <thead> <tr> <th><math>-\Delta U_{B/M}</math> (cal/g)</th> <th><math>-\Delta U_B</math> (kcal/mol)</th> <th><math>-\Delta U_R</math> (kcal/mol @ 1 atm and constant vol.)</th> <th><math>-\Delta H_R</math> (kcal/mol @ 1 atm and constant pressure)</th> </tr> </thead> <tbody> <tr> <td>2,756.20 ± 0.40</td> <td>678.41</td> <td>677.13</td> <td>674.76</td> </tr> </tbody> </table>				$-\Delta U_{B/M}$ (cal/g)	$-\Delta U_B$ (kcal/mol)	$-\Delta U_R$ (kcal/mol @ 1 atm and constant vol.)	$-\Delta H_R$ (kcal/mol @ 1 atm and constant pressure)	2,756.20 ± 0.40	678.41	677.13	674.76								
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$p_{C_J}$ [kbar]	207.9	188 <sup>[8]</sup> 195 (@ 1.55 g cm <sup>-3</sup> , calcd. BKWR) <sup>[13]</sup>  175 (@ 1.48 g cm <sup>-3</sup> , calcd. BKWR) <sup>[13]</sup>  176 (@ 1.55 g cm <sup>-3</sup> , calcd. BKWS) <sup>[13]</sup>  158 (@ 1.48 g cm <sup>-3</sup> , calcd. BKWS) <sup>[13]</sup>	0.145 Mbar <sup>[44]</sup>
VoD [m s <sup>-1</sup> ]	7,276 (@ 1.272 g cm <sup>-3</sup> ; $\Delta H = -386.62 \text{ kJ mol}^{-1}$ )	6,798 (@ 1.55 g cm <sup>-3</sup> ) <sup>[9]</sup> 6,850 (@ 1.55 g cm <sup>-3</sup> ) <sup>[20]</sup> 7,020 (@ 1.55 g cm <sup>-3</sup> , calcd. BKWR) <sup>[13]</sup> 6,780 (@ 1.48 g cm <sup>-3</sup> , calcd. BKWR) <sup>[13]</sup> 6,910 (@ 1.55 g cm <sup>-3</sup> , calcd. BKWS) <sup>[13]</sup> 6,660 (@ 1.48 g cm <sup>-3</sup> , calcd. BKWS) <sup>[13]</sup> 7,400 (@ 1.72 g cm <sup>-3</sup> , (TMD), calcd. empirical, R-P method) <sup>[23]</sup> 8,400 (@ 1.72 g cm <sup>-3</sup> , (TMD), calcd. Aizenshtadt method) <sup>[23]</sup> 7,290 (@ 1.72 g cm <sup>-3</sup> , (TMD), calcd., K-J) <sup>[23]</sup> 6,904 (@ 1.55 g cm <sup>-3</sup> , calcd. empirical, Xiong method) <sup>[24]</sup> 7,150 (@ 1.6 g cm <sup>-3</sup> ) <sup>[48]</sup>	6,850 (@ 1.55 g cm <sup>-3</sup> ) <sup>[9,12,13]</sup> 6,850 (@ 1.55 g cm <sup>-3</sup> , 1.0 in charge diameter, pressed, no confinement) <sup>[11]</sup> 6,700 (@ 1.48 g cm <sup>-3</sup> ) <sup>[13]</sup> 4,750 (@ 1.0 g cm <sup>-3</sup> , unconfined charge) <sup>[16]</sup> 7,040 (@ 1.60 g cm <sup>-3</sup> , unconfined charge) <sup>[16]</sup> 6,850 (@ 1.55 g cm <sup>-3</sup> ) <sup>[25]</sup> 7,000 (@ 1.6 g cm <sup>-3</sup> ) <sup>[21]</sup> 6,552 (based on sand test) <sup>[21]</sup> 6,775 (@ 1.55 g cm <sup>-3</sup> , average lit. value) <sup>[21]</sup> 23,100 ft/s (@ 1.5 g/mL) <sup>[36]</sup> 6,500 (@ 1.45 g cm <sup>-3</sup> ) <sup>[38]</sup> 7,150 (F@ 1.63 g cm <sup>-3</sup> ) <sup>[43]</sup>
$V_0$ [L kg <sup>-1</sup> ]	680		909 <sup>[1,14]</sup>

Powdery sample detonated in thin-walled Pb tubes with 12.5 mm diameter<sup>[20]</sup>:

$\rho$ (g cm <sup>-3</sup> )	VoD (mm/s @ 25 °C)	VoD (mm/s @ -80 °C)	VoD (mm/s @ -180 °C)
0.86	4,110	4,240	3,920
	4,100	3,960	4,110
	3,850	3,980	—
	4,020 (av.)	4,060 (av.)	4,020 (av.)

VoD of the red and yellow forms of ammonium picrate in steel pipe (35/42 mm)<sup>[27]</sup>:

$\rho$ (g/cm <sup>3</sup> )	VoD (m/s)	
	Yellow form	Red form
0.86	4,380	—
1.11	—	5,155
1.34	5,835	—
1.35	—	5,835
1.49	6,950	—
1.50	—	6,960
1.55	6,995	—
1.56	—	6,995
1.58	—	6,200
1.60	6,030	—

Critical diameter [cm]	>25.4 mm for sample with $\rho = 1.65$ g cm <sup>-3</sup> <sup>[17]</sup> (see also <sup>[57]</sup> )
Trauzl test [cm <sup>3</sup> , % TNT]	330–335 cm <sup>3</sup> <sup>[27]</sup> , 280 <sup>[46]</sup> , 333 <sup>[46]</sup>
Sand test [g]	39.5 g (200 g bomb) <sup>[11,40]</sup> , ~80% TNT <sup>[16]</sup> , 37.5–39.5 g sand crushed, 78–85% TNT <sup>[17]</sup> , ~92% TNT <sup>[18]</sup> , 84–87% TNT <sup>[21]</sup> , 33.7 g sand crushed (1,700 g bomb, 0.4 g sample) <sup>[21]</sup> , not initiated by LA or MF alone in sand test <sup>[37]</sup> , requires a booster charge of 0.06 g tetryl for initiation in sand test <sup>[37]</sup> , 77% TNT <sup>[37]</sup> , 95% TNT if compressed to $\rho = 1.53$ g cm <sup>-3</sup> <sup>[37]</sup>

	Effect of storage on sand test values (*after 3.5 years @ 50 °C; **after 3.5 years @ 50 °C and 2 years @ magazine temperature) <sup>[11]</sup> :				
Storage	Minimum detonating charge			Sand crushed (g)	
Years	°C	Mercury fulminate (g)	Tetryl (g)		
0			0.06	23	
3.5	50	0.25		23	
2*	Normal		0.03	23	
4*	Normal		0.04	23	
2**	50	0.24		23	
Initiating efficiency	0.20 g LA minimum detonating charge <sup>[11,44]</sup> , 0.06 g tetryl minimum detonating charge <sup>[11]</sup> , min. initiating charge (g) of primary explosive necessary to detonate 0.4 g ammonium picrate (compressed in donor capsules under 1,000 lb/in <sup>2</sup> pressure) <sup>[29]</sup> : 0.8–0.9 g fulminate (with reinforcing cap) <sup>[29]</sup> , 0.30 g HMTD (with reinforcing cap) <sup>[29]</sup> , 0.30 g HMTD (without reinforcing cap) <sup>[29]</sup> , 0.15 g cyanuric azide (pressed with $p = 200 \text{ atm/in}^2$ ) <sup>[29]</sup> , 0.85 g MF (pressed with $p = 200 \text{ atm/in}^2$ ) <sup>[29]</sup> , not detonated by fulminate <sup>[38]</sup> , 0.86 g MF minimum charge to initiate 0.4 g ammonium picrate loaded @ 200 atm pressure <sup>[17]</sup> , not completely detonated by LA of MF and 0.06 g tetryl is required as booster charge <sup>[17]</sup>				
	Effect of moisture on sensitivity to initiation <sup>[17]</sup> :				
% moisture present	Minimum detonating charge of tetryl required (g)				
0.5	0.09				
1.0	0.11				
2.0	0.14				
	Storage of yellow or red forms @ 50 °C for 2 years increases sensitivity and initiation by only MF is possible <sup>[17]</sup> , subsequent storage of yellow form @ magazine temperature for 2 years results in desensitization and a tetryl booster charge is required <sup>[17]</sup> , storage @ magazine temperature for 4 years returns the original sensitivity <sup>[17]</sup> , storage of the red form @ 50 °C has the same effect on sensitivity, but subsequent storage @ magazine temperature for 4 years results in an increase of minimum detonating charge of MF from 0.23 to 0.29 g <sup>[17]</sup>				
	0.4 g = minimum detonating charge of LA required to shock-initiate explosive D <sup>[51]</sup> , minimum priming charge: $\rho = 1.646 \text{ g cm}^{-3}$ , $W_{50}$ (minimum priming weight) = 1,790 mg <sup>[57]</sup>				

Ballistic mortar test	99% TNT <sup>[11,16,18,40]</sup>																																																		
Ballistic pendulum test	98% TNT <sup>[17,37]</sup>																																																		
US NOL gap test	Gap value = 3.81 cm (@ 1.593 g cm <sup>-3</sup> , pressed sample) <sup>[20]</sup>																																																		
LSGT [cm]	<p>37 mm (NOL)<sup>[31]</sup>, 42 mm (LANL)<sup>[31]</sup></p> <p><math>L_g = 169 \times 10^2</math> in (@ 1.604 g cm<sup>-3</sup>, 93.4% TMD, pressed, LASL LSGT)<sup>[32]</sup>,</p> <p><math>L_g = 168 \times 10^2</math> in (@ 1.64 g cm<sup>-3</sup>, 95.4% TMD, pressed, LASL LSGT)<sup>[32]</sup>,</p> <p><math>L_g = 167 \times 10^2</math> in (@ 1.668 g cm<sup>-3</sup>, 97.1% TMD, pressed, LASL LSGT)<sup>[32]</sup>,</p> <p><math>L_g = 160 \times 10^2</math> in (@ 1.60 g cm<sup>-3</sup>, 93.2% TMD, pressed, NSWC LSGT)<sup>[32]</sup>,</p> <p><math>L_g = 156 \times 10^2</math> in (@ 1.64 g cm<sup>-3</sup>, 95.1% TMD, pressed, NSWC LSGT)<sup>[32]</sup>,</p> <p><math>L_g = 151 \times 10^2</math> in (extrapolated, NSWC LSGT)<sup>[32]</sup></p> <p><math>H</math>=hydraulic press., data from<sup>[45]</sup>:</p> <table border="1"> <thead> <tr> <th rowspan="2"><math>\rho</math> (g/cm<sup>3</sup>)</th> <th rowspan="2">% TMD</th> <th colspan="2">50% point</th> <th rowspan="2">Particle size (<math>\mu\text{m}</math>)</th> <th rowspan="2">remarks</th> </tr> <tr> <th>Cards</th> <th>kbar</th> </tr> </thead> <tbody> <tr> <td>1.59 <math>H</math></td> <td>92.6</td> <td>150</td> <td>(36)</td> <td>185</td> <td>Ambient <math>T</math></td> </tr> <tr> <td>1.35 <math>H</math></td> <td>78.7</td> <td>177</td> <td>27</td> <td>720</td> <td>Production lot</td> </tr> <tr> <td>1.46 <math>H</math></td> <td>84.6</td> <td>171</td> <td>30</td> <td>720</td> <td>Production lot</td> </tr> <tr> <td>1.53 <math>H</math></td> <td>89.0</td> <td>163</td> <td>31</td> <td>720</td> <td>Yorktown sample</td> </tr> <tr> <td>1.55 <math>H</math></td> <td>90.0</td> <td>169</td> <td>30</td> <td>720</td> <td>Production lot</td> </tr> <tr> <td>1.60 <math>H</math></td> <td>93.2</td> <td>160</td> <td>34</td> <td>720</td> <td>Production lot</td> </tr> <tr> <td>1.64 <math>H</math></td> <td>95.1</td> <td>156</td> <td>36</td> <td>720</td> <td>Production lot</td> </tr> </tbody> </table>	$\rho$ (g/cm <sup>3</sup> )	% TMD	50% point		Particle size ( $\mu\text{m}$ )	remarks	Cards	kbar	1.59 $H$	92.6	150	(36)	185	Ambient $T$	1.35 $H$	78.7	177	27	720	Production lot	1.46 $H$	84.6	171	30	720	Production lot	1.53 $H$	89.0	163	31	720	Yorktown sample	1.55 $H$	90.0	169	30	720	Production lot	1.60 $H$	93.2	160	34	720	Production lot	1.64 $H$	95.1	156	36	720	Production lot
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5 s explosion $T$ [°C]	318 <sup>[11,17,18]</sup> , 318 (dec., cook-off) <sup>[44]</sup> , 318 (open cup) <sup>[51]</sup>
5 s ignition $T$ [°C]	318 (dec., US value) <sup>[20]</sup> , 318 (Russian value) <sup>[20]</sup>
Initiation $T$ [°C]	257–259 (@ 20 °C/min) <sup>[27]</sup>
Detonating $T$ [°C]	318 <sup>[36]</sup> , may detonate if heated to 205 °C <sup>[36]</sup> , 318 (5 s) <sup>[40]</sup> , 290 <sup>[43]</sup>
Explosion $T$ [°C]	318 <sup>[37]</sup> , 405 (0.1 s, no cap used) <sup>[11,17]</sup> , 367 (1 s) <sup>[11,17]</sup> , 318 (5 s) <sup>[17]</sup> , 314 (10 s) <sup>[11,17]</sup> , 299 (15 s) <sup>[11,17]</sup> , 295 (20 s) <sup>[11,17]</sup>
100 °C heat test [% mass loss]	0.1% in first 48 h <sup>[11,17]</sup> , 0.1% in second 48 h <sup>[11,17]</sup> , no explosions in 100 h <sup>[11,17]</sup>
130 °C heat test [% mass loss]	No acidity or explosion in 300 min <sup>[17]</sup>
Vacuum stability test [cm <sup>3</sup> /h]	0.2 cm <sup>3</sup> (g) per 5 g sample @ 100 °C in 40 h <sup>[16]</sup> , 0.4 cm <sup>3</sup> (g) per 5 g sample @ 120 °C in 40 h <sup>[16]</sup> , 0.4 cm <sup>3</sup> (g) per 5 g sample @ 150 °C in 40 h <sup>[16]</sup> , 0.2 cm <sup>3</sup> (g) per 1 g sample @ 100 °C in 40 h <sup>[16]</sup> , 0.4 cm <sup>3</sup> (g) per 1 g sample @ 120 °C in 40 h <sup>[16]</sup> , 0.4 cm <sup>3</sup> (g) per 1 g sample @ 150 °C in 40 h <sup>[16]</sup> , 0.2 cc/40 h @ 100 °C <sup>[11,17]</sup> , 0.4 cc/40 h @ 120 °C <sup>[11,17]</sup> , 0.4 cc/40 h @ 150 °C <sup>[11,17]</sup> , 0.4 cm <sup>3</sup> @ 120 °C, 40 h <sup>[44]</sup> , 0.4 mL, 40 h @ 120 °C <sup>[51]</sup>
Thermal stability	No deterioration on storage @ RT for 20 years <sup>[17]</sup> , no deterioration after storage @ 50 °C for 5+ years <sup>[17]</sup> , no change after magazine storage for 20 years <sup>[37]</sup> , storage of yellow or red forms @ 50 °C for 3 years causes significant increase in sensitivity, but subsequent storage for 2–6 years at magazine temperature results in return to original sensitivity <sup>[37]</sup> , storage @ 65 °C for 1 year causes no obvious dec. <sup>[37]</sup> , vigorous dec. with liberation of ammonia @ 220 °C and this reaction also proceeds at lower $T$ <sup>[43]</sup> , can explode if rapidly heated especially if confined <sup>[48]</sup>
Burn rate [mm/s]	Highly flammable, burns readily <sup>[36]</sup>
Specific pressure, $f$	7,200 m (exptl.) <sup>[27]</sup>
Flame sensitivity	Ignites after 8 swings (yellow form) <sup>[27]</sup> , ignites after 12.5 swings (red form) <sup>[27]</sup>
Solubility [g/mL]	Soluble in warm EtOH, acetone <sup>[28]</sup> , dissolves slowly in EtOH and slow separation on standing <sup>[17]</sup> , very slight solubility in Et <sub>2</sub> O <sup>[17]</sup> , slightly soluble in EtOH and in cold H <sub>2</sub> O <sup>[36]</sup> , soluble in hot H <sub>2</sub> O <sup>[36]</sup> , very soluble in hot water <sup>[37]</sup> , slightly soluble in hot acetone or hot EtOH <sup>[37]</sup> , practically insoluble in Et <sub>2</sub> O, ethyl acetate and octyl alcohol <sup>[37]</sup> , readily soluble in boiling water, 74.8 g/100 g H <sub>2</sub> O @ 100 °C <sup>[43]</sup> , insoluble in benzene <sup>[43]</sup> , slightly soluble in water <sup>[48]</sup> , 1 g in 100 mL H <sub>2</sub> O @ 20 °C <sup>[50]</sup> , slightly soluble in EtOH <sup>[50]</sup>

Solubility g/100 cc of solvent<sup>[11,28]</sup>:

T (°C)	Ethyl acetate	EtOH
0	0.290	0.515
10	0.300	0.690
20	0.338	0.850
30	0.380	1.050
40	0.420	1.320
50	0.450	1.890
60	0.500	2.165
70	0.540	2.760
80	0.560	3.620

Values from<sup>[17]</sup>:

Solvent	Solubility (g) in 100 g solvent						
	0 °C	10 °C	20 °C	30 °C	50 °C	80 °C	100 °C
Water	—	0.70	102	—	—	—	75
Ethanol	0.51	0.69	0.86	1.05	1.89	3.62	—
Ethyl acetate	0.29	0.30	0.34	0.38	0.45	0.56	—
Acetone	—	—	—	2.85	—	—	—
Octyl alcohol	—	—	0.2 @ 25 °C	—	—	—	—

Solubility in binary solvent mixtures @ 25 °C (g/100 g solvent after 5 min stirring)<sup>[41]</sup>:

Solvent	Ammonium picrate
DMSO	75
NMP	62
NMP 79.2%, DMSO 20.8%	70
DMF	90
DMF 71.1%, DMSO 28.9%	95

Hygroscopicity	0.1% @ 100% RH <sup>[11]</sup> , moderately hygroscopic <sup>[36]</sup> , not hygroscopic when exposed to humid air but direct contact with moisture should be avoided <sup>[37]</sup> , absorbs moisture <sup>[38]</sup> , hygroscopic – absorbs <5% weight of water on storage in moisture-saturated atmosphere <sup>[40]</sup> , considerably more hygroscopic than PA <sup>[43]</sup> , >5% water absorbed if stored in moist atmosphere for 1 month <sup>[43]</sup>															
Photosensitivity	UV – 0.1% H <sub>2</sub> O <sub>2</sub> static system treatment of aqueous explosive D solns. (500 ppm explosive D) <sup>[26]</sup> :															
	<table border="1"> <thead> <tr> <th>UV exposure time (h)</th><th>ppm H<sub>2</sub>O<sub>2</sub></th><th>TOC analyzer</th></tr> </thead> <tbody> <tr> <td>0</td><td>1,000</td><td>168</td></tr> <tr> <td></td><td>1 ~ 12</td><td>15.6</td></tr> <tr> <td>2</td><td>0</td><td>2.2</td></tr> <tr> <td>5</td><td>0</td><td>–</td></tr> </tbody> </table>	UV exposure time (h)	ppm H <sub>2</sub> O <sub>2</sub>	TOC analyzer	0	1,000	168		1 ~ 12	15.6	2	0	2.2	5	0	–
UV exposure time (h)	ppm H <sub>2</sub> O <sub>2</sub>	TOC analyzer														
0	1,000	168														
	1 ~ 12	15.6														
2	0	2.2														
5	0	–														
Compatibility	Dec. in alkalis <sup>[17]</sup> , compatible with TNT or black powder @ 100 °C <sup>[17]</sup> , reacts with NG, NC, PETN or tetryl @ 100 °C <sup>[17]</sup> , in the presence of moisture reacts readily with lead, steel, nickel-plated steel, slightly with copper-plated steel or zinc-plated steel and bronze <sup>[36]</sup> , when wet it reacts slowly with iron, lead and copper <sup>[36]</sup> , reaction with metals is negligible when dry <sup>[36]</sup> , initiation sensitivity decreases if moist <sup>[37]</sup> , reacts with metals in the presence of moisture <sup>[37]</sup> , absorbs moisture and slowly reacts with metals in wet conditions, for example, Cu and Pb to form dangerous picrate salts <sup>[38]</sup> , does not react with metals when dry <sup>[40]</sup> , reacts with metals to form sensitive metal picrates when wet <sup>[40]</sup> , completely dry ammonium picrate undergoes virtually no reaction with metals and their oxides, whereas moist does, but more slowly than PA does <sup>[43]</sup> , reacts with lead and copper salts to form the corresponding picrates (primary explosives) <sup>[48]</sup> , can form spontaneously explosive ammonium chlorate if in contact with moist potassium chlorate <sup>[48]</sup>															
Susan V-50 test [f/s]	400 (NWL/D) <sup>[31]</sup>															
Susan LVR test [f/s]	990 (NWL/D) <sup>[31]</sup>															
Rifle bullet impact test	30% trials burned, 70% trials unaffected <sup>[11,44]</sup> , three partially burned samples in 10 trials <sup>[17]</sup> , 10 (% detonations, pressed sample, Reg disk bomb, $\frac{3}{16}$ in steel disk) <sup>[55]</sup>															
Plate dent test	Brisance = 91% TNT @ 1.50 g cm <sup>-3</sup> , method A, pressed, confined <sup>[11,17]</sup>															
Fragmentation test	90 mm HE, M71 projectile, lot WC-91: $\rho = 1.50 \text{ g cm}^{-3}$ , charge wt. = 1.94 lb, total no. of fragments for TNT = 703, for subject HE = 649 <sup>[11]</sup> 3 in HE, M42A1 projectile, Lot KC-5: $\rho = 1.55 \text{ g cm}^{-3}$ , charge wt. = 0.82 lb, total no. of fragments for TNT = 514, for subject HE = 508 <sup>[11]</sup> Brisance = 91% TNT (@ 1.50 g cm <sup>-3</sup> ) <sup>[17]</sup> , 96% TNT (@ 1.53 g cm <sup>-3</sup> ) <sup>[17]</sup> , 99% TNT (@ 1.55 g cm <sup>-3</sup> ) <sup>[17]</sup>															

Booster sensitivity test	Condition = pressed, 100 g tetryl, 1.27 in wax for 50% detonation, $\rho = 1.54 \text{ g cm}^{-3}$ <sup>[11,44]</sup> , pressed ammonium picrate, 50% gap = 1.27 in, $\rho = 1.54 \text{ g cm}^{-3}$ <sup>[41]</sup>
Refractive index	1.508 @ 20 °C ( $\alpha$ ) <sup>[17]</sup> , 1.870 @ 20 °C ( $\beta$ ) <sup>[17]</sup> , 1.907 @ 20 °C ( $\gamma$ ) <sup>[17]</sup>

\* No difference in the values of explosive properties of yellow and red ammonium picrate<sup>[27,28]</sup>

	Ammonium picrate <sup>[12,15,17]</sup>	Ammonium picrate <sup>[12,15,17]</sup>	Ammonium picrate <sup>[53]</sup>
	( $\alpha$ -polymorph)	( $\beta$ -polymorph, $T \geq 150$ °C)	
Chemical formula	$\text{C}_6\text{H}_6\text{N}_4\text{O}_7$	$\text{C}_6\text{H}_6\text{N}_4\text{O}_7$	$\text{C}_6\text{H}_6\text{N}_4\text{O}_7$
Molecular weight [g mol <sup>-1</sup> ]	246.14	246.14	246.1
Crystal system	Orthorhombic	Monoclinic	Orthorhombic
Space group	<i>I b c a</i> (no. 73)		<i>I b c a</i> (no. 73)
<i>a</i> [ $\text{\AA}$ ]	13.45	No cell parameters reported	13.474(4)
<i>b</i> [ $\text{\AA}$ ]	19.74		19.790(7)
<i>c</i> [ $\text{\AA}$ ]	7.12		7.131(4)
$\alpha$ [°]	90		90
$\beta$ [°]	90		90
$\gamma$ [°]	90		90
<i>V</i> [ $\text{\AA}^3$ ]			1,901
<i>Z</i>	8		8
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.717		1.72
<i>T</i> [K]			295

Exists as yellow monoclinic crystals in stable form<sup>[37]</sup> and as red rhombic crystals in metastable form<sup>[37]</sup>. These two forms are interconvertible and exhibit the same explosive properties<sup>[37]</sup>; bright red crystalline form when freshly prepared but slowly converts to yellow form on contact with water over several months<sup>[48]</sup>; yellow form is obtained on repeated recryst. from water.<sup>[48]</sup>

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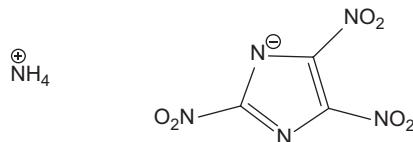
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## Ammonium 2,4,5-trinitroimidazole

Name [German, acronym]: Ammonium 2,4,5-trinitroimidazole, [ammonium-2,4,5-trinitroimidazol, ATNI]

Main (potential) use: explosive

Structural formula:



	<b>ATNI</b>
Formula	C <sub>3</sub> H <sub>4</sub> N <sub>6</sub> O <sub>6</sub>
Molecular mass [g mol <sup>-1</sup> ]	220.10
Appearance at RT	Solid <sup>[1]</sup> , yellow solid <sup>[2]</sup>
IS [J]	50.3 cm (type 12) <sup>[1,4]</sup> , 18% explosion probability (10 kg mass, 250 mm drop height, 50 mg sample, @ 22 °C, 61% ambient humidity, HGZ apparatus) <sup>[2]</sup> , H <sub>50</sub> = 50 cm <sup>[3]</sup> , H <sub>50</sub> = 19 cm (predicted) <sup>[3]</sup> , H <sub>50</sub> = 54 cm (predicted, artificial neural network) <sup>[3]</sup>
FS [N]	2% explosion probability (1.5 kg pendulum weight, 96 ° swing angle, 4.90 MPa gauge pressure, 30 mg sample, 24 °C, 57% ambient humidity, MGY1 apparatus) <sup>[2]</sup>
N [%]	38.18
Ω(CO <sub>2</sub> ) [%]	-14.5
T <sub>m.p.</sub> [°C]	248 <sup>[1]</sup> , 254.52 (endo, peak max, DSC @ 20 °C/min) <sup>[2]</sup> , 249–251 (crude product) <sup>[2]</sup> , 250.5 <sup>[4]</sup>
T <sub>dec.</sub> [°C]	Stable to 248 (DTA) <sup>[1]</sup> , 308.31 (exo, peak max, DSC @ 20 °C/min) <sup>[2]</sup> , 203.6 (mass loss begins, TG @ 20 °C/min, 25% mass loss between 203.6 and 248.4 °C) <sup>[2]</sup> , stable up to 248 (DTA) <sup>[4]</sup>
ρ [g cm <sup>-3</sup> ]	1.825 (crystal) <sup>[1]</sup> , 1.81 <sup>[2]</sup> , 1.835 (crystal) <sup>[4]</sup>
Heat of formation	-86.02 kJ/mol (ΔH <sub>f</sub> °) <sup>[1,4]</sup>
Calcd. (EXPLO5 6.03)	Lit. values
-Δ <sub>ex</sub> U ° [kJ kg <sup>-1</sup> ]	
T <sub>ex</sub> [K]	

$p_{C_J}$ [kbar]		330 ( $\rho$ not specified, calcd.) <sup>[1]</sup>  34.60 GPa (@ 1.81 g cm <sup>-3</sup> , calcd.) <sup>[2]</sup>	
VoD [m s <sup>-1</sup> ]		8,560 ( $\rho$ not specified, calcd.) <sup>[1]</sup>  8,782 (@ 1.81 g cm <sup>-3</sup> , calcd.) <sup>[2]</sup>	
$V_0$ [L kg <sup>-1</sup> ]			
Critical $T$ [°C]	261 (calcd. from kinetics constants) <sup>[4]</sup>		
Thermal stability	Thermally stable up to 248 °C (DTA) <sup>[4]</sup> , no explosions below 262 °C <sup>[4]</sup>		
Vacuum stability test [cm <sup>3</sup> /h]	4.4 cm <sup>3</sup> /g/48 h @ 200 °C <sup>[1,4]</sup> , 5.4 cm <sup>3</sup> /g/29 days @ 175 °C <sup>[1,4]</sup>		
Solubility [g/mL]	Recryst. from ethyl acetate <sup>[1]</sup>		
$\Delta H_{\text{fusion}}$ [cal/mol]	6,705 <sup>[4]</sup>		
Thermal conductivity [cal/cm/s/°C]	$2.5 \times 10^{-4}$ (est.) <sup>[4]</sup>		

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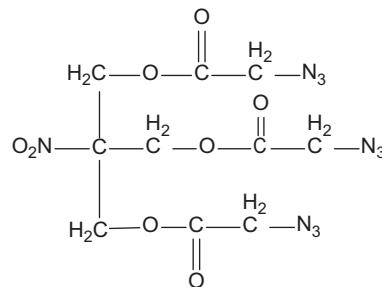
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## Azido-acetic-acid-3-(2'-azido-acetoxy)-2-(2'-azido-acetoxymethyl)-2-nitro-propylester

Name [German, acronym]: Trimethylol nitromethane tris(azidoacetate) [TMNTA]

Main (potential) use: Possible energetic plasticizer<sup>[1]</sup>

Structural formula:



	<b>TMNTA</b>		
Formula	$\text{C}_{10}\text{H}_{12}\text{N}_{10}\text{O}_8$		
Molecular mass [g mol <sup>-1</sup> ]	400.27		
Appearance at RT	Liquid <sup>[1]</sup>		
IS [J]	16 Nm <sup>[1-3]</sup>		
FS [N]	192 <sup>[1-3]</sup>		
N [%]	34.99		
$\Omega(\text{CO}_2)$ [%]	-71.95		
$T_{\text{glass transition}}$ [°C]	-34.1 <sup>[1,2]</sup> , -34.1 (midpoint) <sup>[3]</sup>		
$T_{\text{dec.}}$ [°C]	214 (deflagration point, DSC @ 5 K/min) <sup>[1,3]</sup> , 217.2 (exo, onset, DSC) <sup>[1,3]</sup> , 207.7 (TG) <sup>[1,3]</sup>		
$\rho$ [g cm <sup>-3</sup> ]	1.45 (@ 25 °C) <sup>[1-3]</sup>		
Heat of formation	-240.54 kJ/mol (enthalpy of form.) <sup>[1]</sup> , -230.54 kJ/mol ( $\Delta H_f$ ) <sup>[2]</sup> , -230.54 kJ/mol (enthalpy of form.) <sup>[3]</sup>		
Heat of combustion	5,435.0 kJ/mol <sup>[1,3]</sup>		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^\circ$ [kJ kg <sup>-1</sup> ]			
$T_{\text{ex}}$ [K]			

$p_{CJ}$ [kbar]			
VoD [ $\text{m s}^{-1}$ ]			
$V_0$ [ $\text{L kg}^{-1}$ ]			
<hr/>			
5 s explosion $T$ [ $^{\circ}\text{C}$ ] Deflagration $T$ [ $^{\circ}\text{C}$ ]	214 (DSC @ 5 K/min) <sup>[1,2]</sup>		
Thermal stability	0.25% mass loss @ 90 $^{\circ}\text{C}$ , ca. 80 days <sup>[1-3]</sup>		
Viscosity [ $\text{mPa s}$ ]	1,288 @ 20 $^{\circ}\text{C}$ <sup>[1,3]</sup> , 749 @ 25 $^{\circ}\text{C}$ <sup>[1,3]</sup> , 1,288 <sup>[2]</sup>		
Dutch test	0.24% (110 $^{\circ}\text{C}$ , 72 h) <sup>[1,3]</sup>		

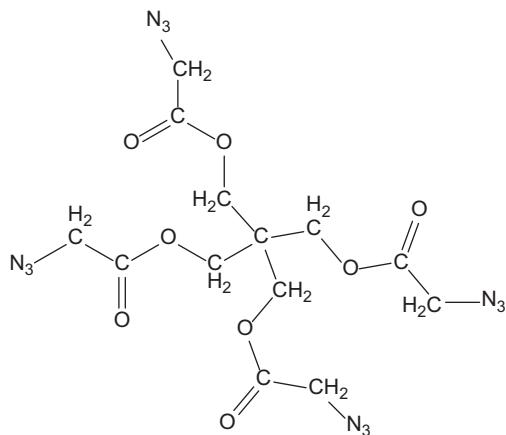
- [1] D. Drees, D. Löffel, A. Messmer, K. Schmid, *Synthesis and Characterization of Azido Plasticizer*, ICT 2000, Karlsruhe, Germany, pp. 52-1–52-12.
- [2] A. Provatas, *Energetic Polymers and Plasticizers for Explosive Formulations – A Review of Recent Advances*, DSTO-TR-0966, DSTO, Melbourne, Australia, April 2000.
- [3] D. Drees, D. Löffel, A. Messmer, K. Schmid, *Propellants, Explosives, Pyrotechnics*, 1999, 24, 159–162.

**Azido-acetic-acid-3-(2'-azido-acetoxy)-2,2-bis-(2'-azido-acetoxymethylpropylester)**

Name [German, acronym]: Azido-acetic-acid-3-(2'-azido-acetoxy)-2,2-bis-(2'-azido-acetoxymethylpropylester) [PETKAA]

Main (potential) use: Energetic plasticizer

Structural formula:



	PETKAA
Formula	$\text{C}_{13}\text{H}_{16}\text{N}_{12}\text{O}_8$
Molecular mass [g mol <sup>-1</sup> ]	468.35
Appearance at RT	Liquid <sup>[1]</sup>
IS [J]	60 Nm <sup>[1-3]</sup>
FS [N]	360 <sup>[1-3]</sup>
N [%]	35.89
$\Omega(\text{CO}_2)$ [%]	-88.82
$T_{\text{glass transition}}$ [°C]	-35.4 (midpoint) <sup>[1,3]</sup> , -35.4 <sup>[2]</sup>
$T_{\text{dec.}}$ [°C]	221.5 (onset, DSC) <sup>[1,3]</sup> , 218.0 (TG) <sup>[1]</sup> , 212.0 (TG) <sup>[3]</sup>
$\rho$ [g cm <sup>-3</sup> ]	1.39 (@ 25 °C) <sup>[1,3]</sup> , 1.39 <sup>[2]</sup>
Heat of formation	-215.20 kJ/mol (enthalpy of form.) <sup>[1-3]</sup>
Heat of combustion	7,202.0 kJ/mol <sup>[1,3]</sup>

	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{\text{ex}} U^\circ [\text{kJ kg}^{-1}]$			
$T_{\text{ex}} [\text{K}]$			
$p_{\text{C-J}} [\text{kbar}]$			
$\text{VoD} [\text{m s}^{-1}]$			
$V_0 [\text{L kg}^{-1}]$			
5 s explosion $T [\text{°C}]$ Deflagration point $[\text{°C}]$	234 (@ 5 K/min) <sup>[1-3]</sup>		
Viscosity [ $\text{mPa s}$ ]	2,880 @ 20 $^{\circ}\text{C}$ <sup>[1,3]</sup> , 1,612 @ 25 $^{\circ}\text{C}$ <sup>[1,3]</sup> , 2,880 <sup>[2]</sup>		
Dutch test	0.57% (110 $^{\circ}\text{C}$ , 72 h) <sup>[1,3]</sup>		

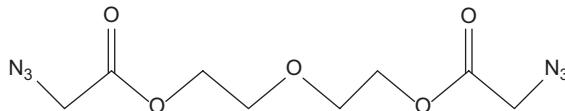
- [1] D. Drees, D. Löffel, A. Messmer, K. Schmid, *Synthesis and Characterization of Azido Plasticizer*, ICT 2000, Karlsruhe, Germany, pp. 52-1–52-12.
- [2] A. Provatas, *Energetic Polymers and Plasticizers for Explosive Formulations – A Review of Recent Advances*, DSTO-TR-0966, DSTO, Melbourne, Australia, April 2000.
- [3] D. Drees, D. Löffel, A. Messmer, K. Schmid, *Propellants, Explosives, Pyrotechnics*, 1999, 24, 159–162.

### Azido-acetic-acid-2-[2'-(2"-azido-acetoxy)-ethoxy]-ethylester

Name [German, acronym]: Azido-acetic-acid-2-[2''-(2''-azido-acetoxy)-ethoxy]-ethylester, [DEGBA, DEGBAA]

Main (potential) use: Energetic plasticizer<sup>[1]</sup>

Structural formula:



5 s explosion $T$ [ $^{\circ}$ C] Deflagration point [ $^{\circ}$ C]	235 (DSC @ 5 K/min) <sup>[1-3]</sup>
Thermal stability	0.48% mass loss after ~80 days @ 90 $^{\circ}$ C <sup>[2,3]</sup>
Viscosity [mPa s]	29.2 (@ 20 $^{\circ}$ C) <sup>[1,3]</sup> , 29.2 <sup>[2]</sup>
Dutch test	0.14% (110 $^{\circ}$ C, 72 h) <sup>[1,3]</sup>
Weight loss	0.48% (90 $^{\circ}$ C, ca. 80 days) <sup>[1]</sup>

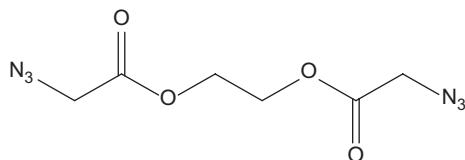
- [1] D. Drees, D. Löffel, A. Messmer, K. Schmid, *Synthesis and Characterization of Azido Plasticizer*, ICT 2000, Karlsruhe, Germany, pp. 52-1–52-12.
- [2] A. Provatas, *Energetic Polymers and Plasticizers for Explosive Formulations – A Review of Recent Advances*, DSTO-TR-0966, DSTO, Melbourne, Australia, April 2000.
- [3] D. Drees, D. Löffel, A. Messmer, K. Schmid, *Propellants, Explosives, Pyrotechnics*, 1999, 24, 159–162.

## Azido-acetic-acid-2-(2'-azido-acetoxy)-ethylester

Name [German, acronym]: Ethylene glycol bis(azidoacetate) ester [EGBAA]

Main (potential) use: Energetic plasticizer<sup>[1]</sup>

Structural formula:



	<b>EGBAA</b>																					
Formula	C <sub>6</sub> H <sub>8</sub> N <sub>6</sub> O <sub>4</sub>																					
Molecular mass [g mol <sup>-1</sup> ]	228.17																					
Appearance at RT	Liquid <sup>[1]</sup>																					
IS [J]	5.5 Nm <sup>[1,3,5]</sup> , 79.4% (2 kg mass) <sup>[2]</sup>																					
FS [N]	165 <sup>[1,3,5]</sup> , 0% (relative pressure = 2.5 MPa, pendulum angle = 66 °) <sup>[2]</sup>																					
N [%]	36.83																					
Ω(CO <sub>2</sub> ) [%]	-84.15																					
T <sub>glass transition point</sub> [°C]	-69.05 <sup>[2]</sup> , -70.8 <sup>[3]</sup> , -69.4 <sup>[4]</sup> , -70.8 (midpoint) <sup>[5]</sup> , -66.7 (midpoint, with 50% polyNIMMO, DSC @ 10 °C/min) <sup>[5]</sup>																					
T <sub>dec.</sub> [°C]	227.4 (onset), 252.05 (peak max.) (DSC @ 10 °C/min, 1 mg sample, N <sub>2</sub> flow) <sup>[2]</sup> , TG-DTG (@ 10 °C/min) shows two-stage mass loss process: stage 1 onset @ 83.58 °C, completed @ 195.17 °C (59.70% mass loss), stage 2 completed @ 225.01 °C (38.59% mass loss) <sup>[2]</sup> , 206.4 (onset, DSC) <sup>[5]</sup> , 218.0 (TG) <sup>[5]</sup>  Initial T(T <sub>0</sub> ) and max. peak T(T <sub>p</sub> ) of exothermic dec. @ different heating rates <sup>[2]</sup> :  <table border="1"> <thead> <tr> <th>β (K/min)</th> <th>5</th> <th>10</th> <th>15</th> <th>20</th> <th>30</th> <th>40</th> </tr> </thead> <tbody> <tr> <td>T<sub>0</sub> (K)</td> <td>439.25</td> <td>443.85</td> <td>445.55</td> <td>449.05</td> <td>456.15</td> <td>466.05</td> </tr> <tr> <td>T<sub>p</sub> (K)</td> <td>515.15</td> <td>525.2</td> <td>527.85</td> <td>533.85</td> <td>540.85</td> <td>545.255</td> </tr> </tbody> </table>	β (K/min)	5	10	15	20	30	40	T <sub>0</sub> (K)	439.25	443.85	445.55	449.05	456.15	466.05	T <sub>p</sub> (K)	515.15	525.2	527.85	533.85	540.85	545.255
β (K/min)	5	10	15	20	30	40																
T <sub>0</sub> (K)	439.25	443.85	445.55	449.05	456.15	466.05																
T <sub>p</sub> (K)	515.15	525.2	527.85	533.85	540.85	545.255																
ρ [g cm <sup>-3</sup> ]	1.34 <sup>[1-3]</sup> , 1.18 <sup>[4]</sup> , 1.34 (@ 25 °C) <sup>[5]</sup>																					
Heat of formation	-167.38 kJ/mol (enthalpy of formation) <sup>[1,5]</sup> , -167.36 kJ/mol (ΔH <sub>f</sub> ) <sup>[3]</sup>																					

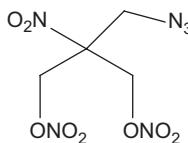
Heat of combustion	3,344.3 kJ/mol <sup>[1,5]</sup>		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^\circ [\text{kJ kg}^{-1}]$		Heat of detonation = 1,065 J/g <sup>[2]</sup>	
$T_{\text{ex}} [\text{K}]$			
$p_{\text{CJ}} [\text{kbar}]$			
$\text{VoD} [\text{m s}^{-1}]$			
$V_0 [\text{L kg}^{-1}]$			
Critical $T$ of thermal explosion [°C]	248.29 <sup>[2]</sup>		
5 s explosion $T$ [°C] Deflagration point [°C]	232 (DSC @ 5 K/min) <sup>[1,3,5]</sup> , 201.5 (@ 2 °C/min, with 50% polyNIMMO) <sup>[5]</sup>		
Thermal stability	0.9% mass loss @ 90 °C for ~ 80 days <sup>[1,3,5]</sup>		
Viscosity [mPa s]	23.4 (@ 20 °C) <sup>[1,5]</sup> , 19.3 (@ 25 °C) <sup>[1,2,5]</sup> , 23.4 <sup>[3]</sup> , 0.399 (with 50% polyNIMMO) <sup>[5]</sup>		
Dutch test	0.26% (110 °C, 72 h) <sup>[1,5]</sup> , 0.60% (105 °C, 72 h, ≤2%, with 50% polyNIMMO) <sup>[5]</sup>		
$\Delta H_{\text{dec}}$ [J/g]	1,029 <sup>[2]</sup>		

- [1] D. Drees, D. Löffel, A. Messmer, K. Schmid, *Synthesis and Characterization of Azido Plasticizer*, ICT 2000, Karlsruhe, Germany, pp. 52-1–52-12.
- [2] H.-X. Gao, F.-Q. Zhao, R.-Z. Hu, H. Zhang, S.-Y. Xu, J.-H. Yi, Y. Gao, W. Wang, Y.-P. Ji, *Non-Isothermal Decomposition Reaction Kinetics of Azido-Acetic-Acid-2-(2-azido-acetoxy)-ethylester (EGBAA)*, ICT 2007, Karlsruhe, Germany, pp. 61-1–61-12.
- [3] A. Provatas, *Energetic Polymers and Plasticizers for Explosive Formulations – A Review of Recent Advances*, DSTO-TR-0966, DSTO, Melbourne, Australia, April 2000.
- [4] 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.
- [5] D. Drees, D. Löffel, A. Messmer, K. Schmid, *Propellants, Explosives, Pyrotechnics*, 1999, 24, 159–162.

## Azidomethyl-dinitroxydimethyl-nitromethane

Name [German, acronym]: Azidomethyl-dinitroxydimethyl-nitromethane,  
 [azidomethyl-dinitroxydimethyl-nitromethan,  
 AMDNNM]

Main (potential) use: Possible new energetic plasticizer  
 Structural formula:



	AMDNNM		
Formula	$\text{C}_4\text{H}_6\text{N}_6\text{O}_8$		
Molecular mass [g mol <sup>-1</sup> ]	266.13		
Appearance at RT	Yellow oil, liquid <sup>[1]</sup>		
IS [J]	$H_{50\%} = 6.8 \text{ cm}$ (2.5 kg mass, LANL type 12, Bruceton method) <sup>[1]</sup>		
FS [N]	>36.7 kg (BAM, 50% load) <sup>[1]</sup>		
ESD [J]	0.025 (ABL) <sup>[1]</sup>		
N [%]	31.58		
$\Omega(\text{CO}_2)$ [%]	-18.0		
$T_{\text{glass transition}}$ [°C]	0–5 (DSC @ 10 °C/min, 1 mg, Al pan with pinhole lid) <sup>[1]</sup>		
$T_{\text{dec.}}$ [°C]	151 (onset), 197 (exo peak max) (DSC @ 10 °C/min, 1 mg, Al pan with pinhole lid) <sup>[1]</sup>		
$\rho$ [g cm <sup>-3</sup> ]	1.55 (flootation) <sup>[1]</sup>		
Heat of formation	17.51 kJ/mol (est., calcd.) <sup>[1]</sup>		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^\circ$ [kJ kg <sup>-1</sup> ]			
$T_{\text{ex}}$ [K]			
$p_{\text{C-J}}$ [kbar]		25 GPa (@ 1.55 g cm <sup>-3</sup> , calcd., CHEETAH) <sup>[1]</sup>	
VoD [m s <sup>-1</sup> ]		7,860 (@ 1.55 g cm <sup>-3</sup> , calcd., CHEETAH) <sup>[1]</sup>	

$V_0$ [L kg <sup>-1</sup> ]			
Vapor pressure [atm @ °C]	Nonvolatile liquid @ RT <sup>[1]</sup>		
Solubility [g/mL]	Soluble in acetone <sup>[1]</sup>		
$I_{sp}$ [s]	258.31 <sup>[1]</sup>		

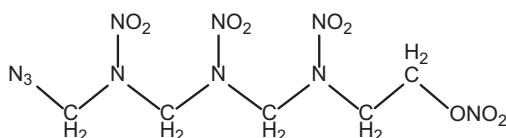
[1] M. C. Schulze, D. E. Chavez, *J. Energet. Mater.*, **2016**, *34*, 129–137.

**1-Azido-8-nitrato-2,4,6-trinitro-2,4,6-triazaoctane**

Name [German, acronym]: 1-Azido-8-nitrato-2,4,6-trinitro-2,4,6-triazaoctane,  
 [1-azido-8-nitrato-2,4,6-trinitro-2,4,6-triazaoctan,  
 ANTTO]

Main (potential) use: decomp. temp. too low

Structural formula:



	ANTTO		
Formula	C <sub>5</sub> H <sub>10</sub> N <sub>10</sub> O <sub>9</sub>		
Molecular mass [g mol <sup>-1</sup> ]	354.20		
Appearance at RT			
IS [J]	4 (40 cm drop height, 1 kg mass) <sup>[1]</sup>		
FS [N]	120 (crackling) <sup>[1]</sup>		
N [%]	39.55		
Ω(CO <sub>2</sub> ) [%]	-27.1		
T <sub>m.p.</sub> [°C]	111 (DSC @ 5 K/min) <sup>[1]</sup>		
T <sub>dec.</sub> [°C]	132 (DSC @ 5 K/min) <sup>[1]</sup>		
ρ [g cm <sup>-3</sup> ]			
Heat of formation			
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
-Δ <sub>ex</sub> U° [kJ kg <sup>-1</sup> ]			
T <sub>ex</sub> [K]			
p <sub>C,J</sub> [kbar]			
VoD [m s <sup>-1</sup> ]			
V <sub>0</sub> [L kg <sup>-1</sup> ]			

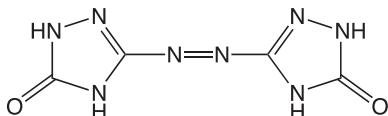
[1] C. Wagner, G. Heeb, T. M. Klapötke, B. Krumm, X. Steemann, J. Weigand, *A New Energetic Material – From the Laboratory Synthesis to the Technical Production*, ICT 2007, Karlsruhe, Germany, pp. 52-1–52-9.

## Azotriazolone

Name [German, acronym]: Azotriazolone [Azotriazolon, AzoTO]

Main (potential) use: Secondary (high) explosive

Structural formula:



	Azotriazolone
Formula	C <sub>4</sub> H <sub>4</sub> N <sub>8</sub> O <sub>2</sub>
Molecular mass [g mol <sup>-1</sup> ]	196.13
Appearance at RT	
IS [J]	15 <sup>a</sup> <sup>[1]</sup>
FS [N]	>360 <sup>[1]</sup>
ESD [J]	Ignition at 0.45 J not at 0.045 J <sup>[1]</sup>
N [%]	57.1
Ω (CO <sub>2</sub> ) [%]	-65.3
T <sub>m.p.</sub> [°C]	>300 (dec.) <sup>[1]</sup>
T <sub>dec.</sub> [°C]	365 (peak) 302 (onset) (DSC @ 10 °C/min) <sup>[1]</sup>
ρ [g cm <sup>-3</sup> ]	1.91 (@ TMD) <sup>[1]</sup>
Heat of formation	155 kJ/mol (ΔH <sub>f</sub> , calcd.) <sup>[1]</sup> , 790.3 kJ kg <sup>-1</sup> (ΔH <sub>f</sub> , calcd.) <sup>[1]</sup>
	Calcd. (CHEETAH 2.0)
	exptl.
-Δ <sub>ex</sub> U° [kJ kg <sup>-1</sup> ]	
T <sub>ex</sub> [K]	
p <sub>C-J</sub> [kbar]	286 <sup>[1]</sup>
VoD [m s <sup>-1</sup> ]	8,021 (@ TMD) <sup>[1]</sup>
V <sub>0</sub> [L kg <sup>-1</sup> ]	

<sup>a</sup> Converted from Rotter F of I = 100 (using a standard of RDX = 80).

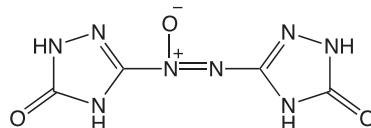
[1] C. J. Underwood, C. Wall, A. Provatas, L. Wallace, *New. J. Chem.*, 2012, 36, 2613–2617.

## Azoxytriazolone

Name [German, acronym]: Azoxytriazolone [Azoxytriazolon, AZTO]

Main (potential) use: Secondary (high) explosive

Structural formula:



	AZTO <sup>a</sup>		
Formula	C <sub>4</sub> H <sub>4</sub> N <sub>8</sub> O <sub>3</sub>		
Molecular mass [g mol <sup>-1</sup> ]	212.13		
Appearance at RT			
IS [J]	9.4 <sup>b [1]</sup> , >50 (AZTO) <sup>[2]</sup>		
FS [N]	>360 <sup>[1]</sup> , >353 (AZTO) <sup>[2]</sup>		
ESD [J]	Ignition at 4.5 J not at 0.45 J <sup>[1]</sup>		
N [%]	52.8		
Ω(CO <sub>2</sub> ) [%]	-52.8		
T <sub>m.p.</sub> [°C]	>300 (dec.) <sup>[1]</sup>		
T <sub>dec.</sub> [°C]	355 (peak), 267 (onset) (DSC @ 10 °C/min) <sup>[1]</sup> , 280 (onset, DSC, AZTO) <sup>[2]</sup>		
ρ [g cm <sup>-3</sup> ]	1.91 (@ TMD) <sup>[1]</sup> , 1.905 (crystallographic) <sup>[2]</sup>		
Heat of formation	81 (ΔH <sub>f</sub> , calcd.) <sup>[1]</sup> , 381.8 (ΔH <sub>f</sub> , calcd.) <sup>[1]</sup> , 11 kJ/mol (enthalpy of form.) <sup>[2]</sup>		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
-Δ <sub>ex</sub> U° [kJ kg <sup>-1</sup> ]	2,275		
T <sub>ex</sub> [K]	2,299	2,673 (@ 1.905 g cm <sup>-3</sup> , calcd., Cheetah 2.0) <sup>[2]</sup>	
p <sub>C-J</sub> [kbar]	243.9	297 (calcd., Cheetah 2.0) <sup>[1]</sup> 27.99 GPa (@ 1.905 g cm <sup>-3</sup> , calcd., Cheetah 2.0) <sup>[2]</sup>	

VoD [ $\text{m s}^{-1}$ ]	8,204 (@ 1.905 g $\text{cm}^{-3}$ ; $\Delta_f H = 11 \text{ kJ mol}^{-1}$ )	8,204 (@ TMD, calcd., Cheetah 2.0) <sup>[1]</sup>  8,062 (@ 1.905 g $\text{cm}^{-3}$ , calcd., Cheetah 2.0) <sup>[2]</sup>	
$V_0 [\text{L kg}^{-1}]$	733		

<sup>a</sup> Data for samples containing 6% AZTO.<sup>b</sup> Converted from Rotter F of  $I = 100$  (using a standard of RDX = 80).

[1] C. J. Underwood, C. Wall, A. Provatas, L. Wallace, *New. J. Chem.*, **2012**, *36*, 2613–2617.

[2] E.-C. Koch, *State of the Art In insensitive Explosives*, MSIAC Workshop on Sensitivity of Energetic Materials, 11th–12th May 2010.

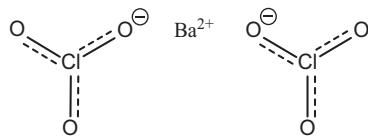
# B

## Barium chlorate

Name [German, acronym]: Barium chlorate [bariumchlorat]

Main (potential) use: Component of pyrotechnical mixtures producing green flames, (historically) oxidizer for the production of green pyrotechnic flames (monohydrate)<sup>[4]</sup>, pyrotechnics (green fire), manufacture of explosives and matches<sup>[5]</sup>

Structural formula:



*Barium chlorate is the anhydrous compound; however, this name is also used widely in the literature to refer to the monohydrate salt.*

	Barium chlorate	
Formula	Ba(ClO <sub>3</sub> ) <sub>2</sub>	
Molecular mass [g mol <sup>-1</sup> ]	304.22 (anhydrous; 324.24, monohydrate)	
Appearance at room temperature (RT)	Colorless crystals or white powder (monohydrate) <sup>[4]</sup> , monohydrate = monoclinic, prismatic crystals <sup>[5]</sup>	
N [%]	0	
Ω(CO <sub>2</sub> ) [%]	+26.3	
T <sub>m.p.</sub> [°C]	414 (dec.) <sup>[2]</sup> , 410 (monohydrate) <sup>[4]</sup> , 414 (but begins to give off oxygen at 250 °C) <sup>[5]</sup>	
T <sub>dehydration</sub> [°C]	120 <sup>[5]</sup>	
T <sub>dec.</sub> [°C]	250 (begins to give off oxygen, but T <sub>m.p.</sub> cited as 414 °C) <sup>[5]</sup>	
ρ [g cm <sup>-3</sup> ]	3.179 (@ 298 K) <sup>[2]</sup> , 3.18 <sup>[1]</sup> , 3.18 (monohydrate) <sup>[4]</sup>	
Heat of formation	-1,080 kJ/mol (enthalpy of form., monohydrate) <sup>[4]</sup> , -2,536.0 kJ kg <sup>-1</sup> <sup>[1]</sup>	
	Calcd. (K-J)	Exptl.
-Δ <sub>ex</sub> U <sup>o</sup> [kJ kg <sup>-1</sup> ]		

$T_{\text{ex}}$ [K]		
$p_{\text{CJ}}$ [GPa]		
VoD [ $\text{m s}^{-1}$ ]		
$V_0$ [L kg $^{-1}$ ]		

Solubility [g/mL]	38 g/100 g H <sub>2</sub> O @ 25 °C (monohydrate) <sup>[4]</sup> , freely soluble in water <sup>[5]</sup> , soluble in hydrochloric acid <sup>[5]</sup> , moderately soluble in ethylamine <sup>[5]</sup> , very sparingly soluble in EtOH but slightly more soluble in acetone <sup>[5]</sup> , essentially insoluble in ethyl acetate, pyridine <sup>[5]</sup>
Compatibility	Fire hazard in contact with combustible material <sup>[5]</sup>

	Barium chlorate <sup>[3]</sup>
Chemical formula	BaCl <sub>2</sub> O <sub>6</sub>
Molecular weight [g mol $^{-1}$ ]	304.22
Crystal system	Orthorhombic
Space group	<i>F d d 2</i> (no. 43)
$a$ [\mathring{A}]	13.273(1)
$b$ [\mathring{A}]	11.774(1)
$c$ [\mathring{A}]	7.7184(9)
$\alpha$ [°]	90
$\beta$ [°]	90
$\gamma$ [°]	90
$V$ [\mathring{A} $^3$ ]	1206.2009
$Z$	8
$\rho_{\text{calc}}$ [g cm $^{-3}$ ]	
$T$ [K]	

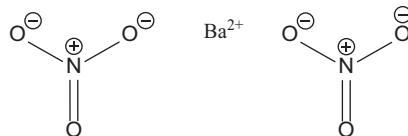
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## Barium nitrate

Name [German, acronym]: Barium nitrate [bariumnitrat, BN]

Main (potential) use: Component in green-flame pyrotechnics and ignition mixtures<sup>[1]</sup>, in some primer compositions and propellants, component of some blasting explosives, oxidizer in composite explosives and pyrotechnics<sup>[8]</sup>, common pyrotechnic oxidizer and green-color flame agent<sup>[10]</sup>, pyrotechnics for green fire, green signal lights<sup>[12]</sup>

Structural formula:



	BN	
Formula	Ba(NO <sub>3</sub> ) <sub>2</sub>	
Molecular mass [g mol <sup>-1</sup> ]	261.34	
Appearance at RT	Colorless crystals or white powder <sup>[9]</sup> , crystals or crystalline powder <sup>[12]</sup>	
N[%]	10.72	
Ω(CO <sub>2</sub> ) [%]	+36.7	
T <sub>m.p.</sub> [°C]	588 <sup>[2]</sup> , 592 <sup>[1,14]</sup> , 575 <sup>[9]</sup> , 590 <sup>[10]</sup> , ~590 <sup>[12]</sup>	
T <sub>dec.</sub> [°C]	685 (TG/DTA @ 10 °C/min) <sup>[2]</sup> , DTA @ 15 °C/min: 588 (fusion), 605 (slight bubbling), 661 (slight NO <sub>2</sub> fumes), 692 (rapid nitrous fumes) <sup>[5]</sup> , mpt. = ~590 °C with dec. at higher temperature <sup>[12]</sup>	
ρ [g cm <sup>-3</sup> ]	3.24 (@ 296.15 K) <sup>[3]</sup> , 3.24 <sup>[4,10,12]</sup> , 3.244 (@ 23 °C) <sup>[8]</sup> , sp. gr. = 3.244 (@ 23 °C) <sup>[9]</sup>	
Heat of formation	-907.3 kcal/kg (enthalpy of form.) <sup>[1]</sup> , -3,796.1 kJ kg <sup>-1</sup> (enthalpy of form.) <sup>[1]</sup> , -3,794.9 kJ/kg <sup>[4]</sup> , -992 kJ/mol (enthalpy of form.) <sup>[10]</sup> , -238.23 kcal/mol ( $\Delta H_f^\circ$ ) <sup>[13]</sup>	
	Calcd. (K-J)	Exptl.
-Δ <sub>ex</sub> U <sup>o</sup> [kJ kg <sup>-1</sup> ]		
T <sub>ex</sub> [K]		

$p_{C_J}$ [GPa]		14 GPa (@ 2.61 g cm <sup>-3</sup> , Baratol with 76 wt.% BN, 24 wt.% TNT) <sup>[13]</sup>
VoD [m s <sup>-1</sup> ]		4925 (2.61 g cm <sup>-3</sup> , Baratol with 76 wt.% BN, 24 wt.% TNT) <sup>[13]</sup>
$V_0$ [L kg <sup>-1</sup> ]		

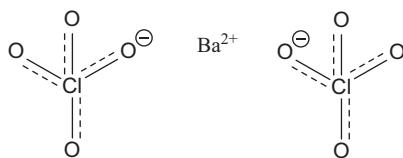
LSGT [cm]	$G_{50} = 27.3$ mm, $L_{95} = 0.20$ mm @ 2.957 g cm <sup>-3</sup> , Baratol with 76 wt.% BN, 24 wt.% TNT <sup>[13]</sup>
SSGT [cm]	no data because sample was below failure diameter (Baratol with 76 wt.% BN, 24 wt.% TNT) <sup>[13]</sup>
Solubility [g/mL]	10 g/100 g H <sub>2</sub> O @ 25 °C <sup>[10]</sup> , freely soluble in H <sub>2</sub> O <sup>[12]</sup> , very slightly soluble in EtOH, acetone <sup>[12]</sup> , 8.7 g/100 g H <sub>2</sub> O @ 20 °C <sup>[13]</sup>
Hygroscopicity	Critical huimidity = 97.7% RH @ 20 °C <sup>[11]</sup>

	Barium nitrate <sup>[6]</sup>	Barium nitrate <sup>[7]</sup>
		(neutron diffraction)
Chemical formula	BaN <sub>2</sub> O <sub>6</sub>	BaN <sub>2</sub> O <sub>6</sub>
Molecular weight [g mol <sup>-1</sup> ]	261.34	261.34
Crystal system	Cubic	Cubic
Space group	Pa3 (no. 205)	P 2 <sub>1</sub> 3 (no. 198)
$a$ [\AA]	8.1184(2)	8.126
$b$ [\AA]	8.1184(2)	8.126
$c$ [\AA]	8.1184(2)	8.126
$\alpha$ [°]	90	90
$\beta$ [°]	90	90
$\gamma$ [°]	90	90
$V$ [\AA <sup>3</sup> ]	533.07	536.58
$Z$	4	
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	3.24	
$T$ [K]		

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## Barium perchlorate

Name [German, acronym]: Barium perchlorate [bariumperchlorat]  
 Main (potential) use: component of pyrotechnical compositions<sup>[1]</sup>  
 Structural formula:



	Barium perchlorate	
Formula	Ba(ClO <sub>4</sub> ) <sub>2</sub>	
Molecular mass [g mol <sup>-1</sup> ]	336.22	
Appearance at RT	White crystals (anhydrous) or colorless liquid if exposed to air (is extremely hygroscopic) <sup>[7]</sup> , trihydrate crystals <sup>[8]</sup>	
N [%]	0	
Ω(CO <sub>2</sub> ) [%]	+19.0 (BaO, HCl), +38.1 (for trihydrate)	
T <sub>phase transition</sub> [°C]	284 ( $\alpha$ - $\rightarrow$ $\beta$ ), 360 ( $\beta$ $\rightarrow$ $\gamma$ ) (DTA @ 15 °C/min) <sup>[5]</sup>	
T <sub>m.p.</sub> [°C]	487 <sup>[2]</sup> , 295 (phase transition), 378 (phase transition) 485–500 (sharp exotherm) (DTA) <sup>[5]</sup> , 284 (alpha $\rightarrow$ beta phase transition), 360 (phase transition to gamma) <sup>[5]</sup> , 505 (dec.) <sup>[5]</sup> ; 469 (fusion), 504 (vigorous dec.) (DTA @ 15 °C/min) <sup>[4]</sup>	
T <sub>dec.</sub> [°C]	507 <sup>[2]</sup> , 505 <sup>[1,5]</sup>	
ρ [g cm <sup>-3</sup> ]	3.2 <sup>[1,5]</sup> , 3.681 (@ 25 °C) <sup>[5]</sup>	
Heat of formation	$-796.26 \pm 1.35 \text{ kJ/mol}$ (calcd.) <sup>[3]</sup> , $-2368.27 \pm 4.02 \text{ kJ kg}^{-1}$ (calcd.) <sup>[3]</sup>	
	Calcd. (K-J)	Exptl.
$-\Delta_{\text{ex}} U^{\circ}$ [kJ kg <sup>-1</sup> ]		
T <sub>ex</sub> [K]		
p <sub>CJ</sub> [GPa]		
VoD [m s <sup>-1</sup> ]		
V <sub>0</sub> [L kg <sup>-1</sup> ]		

Solubility [g/mL]	38 g/100 g H <sub>2</sub> O @ 25 °C (monohydrate) <sup>[4]</sup> , soluble in water, MeOH <sup>[8]</sup> , slightly soluble in EtOH, ethyl acetate, acetone <sup>[8]</sup> , practically insoluble in Et <sub>2</sub> O <sup>[8]</sup>
Hygroscopicity	Too hygroscopic to be of use in unbound or aqueous-bound compositions <sup>[7]</sup> , anhydrous barium perchlorate can be used if protected from moisture with, for example, compositions with polymerizing resins <sup>[7]</sup> , anhydrous barium perchlorate readily converted to liquid on exposure to air <sup>[7]</sup>

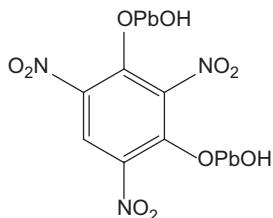
	Barium perchlorate <sup>[6]</sup>
	(α-Polymorph) (X-ray powder diffraction)
Chemical formula	BaCl <sub>2</sub> O <sub>8</sub>
Molecular weight [g mol <sup>-1</sup> ]	336.22
Crystal system	Orthorhombic
Space group	<i>Fdd d</i> (no. 70)
<i>a</i> [Å]	14.304 (9)
<i>b</i> [Å]	11.688 (7)
<i>c</i> [Å]	7.2857 (4)
α [°]	90
β [°]	90
γ [°]	90
<i>V</i> [Å <sup>3</sup> ]	1,218.06
<i>Z</i>	8
<i>ρ</i> <sub>calc</sub> [g cm <sup>-3</sup> ]	
<i>T</i> [K]	

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## Basic lead styphnate

- Name [German, acronym]: Basic lead trinitroresorcinate, basic lead 2,4,6-trinitroresorcinate [basisches bleitrintrioresorcinat, basisches bleistyphnat, basisches blei-2,4,6-trinitroresorcinat, basic LS]
- Main (potential) use: Ingredient of priming compositions<sup>[1,8,12]</sup>, in compositions for high-temperature fuzeheads<sup>[4]</sup>, evaluated for use in primer mixes NOL 60 and NOL 130 (40% basic LS, 20% LA, 2% tetrazene, 15% Sb<sub>2</sub>S<sub>3</sub>, 20% barium nitrate)<sup>[6,8]</sup>, suitable as fast-burning delay composition<sup>[12]</sup>, potential use in electrically initiated trains and as fast-delay composition<sup>[13]</sup>, used in primer mixtures in USA<sup>[13]</sup>, R.D. 1346 tested as ingredient for ammunition priming mixture<sup>[13]</sup>, R.D. 1349 tested as dipping mixture for sensitive fuzeheads<sup>[13]</sup>

Structural formula:



	<b>Basic LS<sup>†</sup></b>
Formula	C <sub>6</sub> H <sub>3</sub> N <sub>3</sub> O <sub>10</sub> Pb <sub>2</sub>
Molecular mass [g mol <sup>-1</sup> ]	691.50
Appearance at RT	Two crystalline forms: yellow crystals or red needles <sup>[1]</sup> , three modifications of the β-polymorph of basic LS have been reported (tan-yellow, RD1346-A; red, RD1346 and tan, RD1349) by altering the crystal habit by the addition of 2-nitroresorcinol <sup>[6]</sup> ; there is also an α-polymorph (tan-brown) which is commercially available <sup>[6]</sup> , two forms: bulky yellow solid consisting of very small particles or red diamond-shaped crystals <sup>[7]</sup> , yellow-tan orthorhombic crystals <sup>[7]</sup> , heavy, red crystalline solid, hexagonal plates (ordinary styphnic acid used in synthesis) <sup>[9]</sup> , yellow crystal needles <sup>[9]</sup> , form and color of basic LS formed depends on the Styphnic acid used <sup>[9]</sup> , exists in at least three polymorphs <sup>[12]</sup> , β-polymorph (red variety) is free-flowing, red-brown crystalline granules <sup>[12]</sup> , α-polymorph is common form of monobasic LS <sup>[13]</sup> , R.D. 1346 and R.D. 1349 both β-polymorphs of monobasic LS, both reduced sensitivity to spark ignition <sup>[13]</sup> , there are three basic LS: yellow acicular crystals (α-form, <i>Böttger</i> and <i>Will</i> ), red diamond-shaped crystals (β-form, <i>Brün</i> ) and amorphous yellow (γ-form, <i>Tauson</i> ) <sup>[13]</sup> , two habit forms of β-polymorph: red rounded granular and oval/cigar-shaped crystals <sup>[13]</sup> , orange solid (tribasic LS dihydrate) <sup>[14]</sup> , orange solid (pentabasic LS dihydrate) <sup>[14]</sup>

IS [J]	$H_{50\%} = 37.3 \pm 11.2$ cm (ball drop IS, steel ball, ball weight = 8.35 g) <sup>[2]</sup> , 96 cm (0.5 kg mass, 34 ± 1 mg sample, ERL machine) <sup>[5]</sup> , 44 cm (1.0 kg mass, 34 ± 1 mg sample, ERL machine) <sup>[5]</sup> , 12 cm (2.5 kg mass, 34 ± 1 mg sample, ERL machine) <sup>[5]</sup> , $H_{10\%} = 8$ in (2 kg mass, P.A.) <sup>[10]</sup> , $H_{50\%} = 14.7$ in (ball drop impact, 7 g steel ball impacting 0.5 mm thick sample layer) <sup>[10]</sup>																											
FS [N]	<p><math>F_{50\%} = 250 \pm 100</math> g (Julius-Peters, BAM, porcelain plate and peg, Bruceton method)<sup>[2]</sup>, <math>F_{10\%} = 40</math> g (Julius-Peters, BAM, porcelain plate and peg, Bruceton method)<sup>[2]</sup></p> <p>Sensitivity to frictional impact (pendulum sensitivity test, pendulum overall length = 20 in, 133 g rod, 364 g steel shoe)<sup>[7]</sup>:</p> <table border="1"> <thead> <tr> <th></th><th>Orthorhombic yellow-tan crystals</th><th>Red, diamond-shaped crystals</th><th>Yellow amorphous</th></tr> </thead> <tbody> <tr> <td>No. of tests</td><td>350</td><td>350</td><td>50</td></tr> <tr> <td>No. firing</td><td>295</td><td>233</td><td>12</td></tr> <tr> <td>No. misfiring</td><td>55</td><td>117</td><td>38</td></tr> </tbody> </table>		Orthorhombic yellow-tan crystals	Red, diamond-shaped crystals	Yellow amorphous	No. of tests	350	350	50	No. firing	295	233	12	No. misfiring	55	117	38											
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ESD [J]	<p>0.000341<sup>[10,15]</sup></p> <p>Approaching electrode electrostatic sensitivity apparatus<sup>[11]</sup>:</p> <table border="1"> <thead> <tr> <th rowspan="2">Discharge</th><th colspan="3">Minimum energy (<math>10^{-7}</math> J)</th></tr> <tr> <th>Approaching needle</th><th>Approaching (pin) plane to plane</th><th>Fixed-gap, parallel plate</th></tr> </thead> <tbody> <tr> <td>Oscillatory</td><td>&lt;2,000</td><td>&lt;830</td><td>4,400</td></tr> <tr> <td>Arc</td><td>70</td><td>-30</td><td>1,100</td></tr> <tr> <td>Spark</td><td>200</td><td>-150w</td><td>900</td></tr> <tr> <td></td><td colspan="3" style="text-align: center;">50% point</td></tr> <tr> <td>Spark</td><td>6,700</td><td>-</td><td>2,600</td></tr> </tbody> </table>	Discharge	Minimum energy ( $10^{-7}$ J)			Approaching needle	Approaching (pin) plane to plane	Fixed-gap, parallel plate	Oscillatory	<2,000	<830	4,400	Arc	70	-30	1,100	Spark	200	-150w	900		50% point			Spark	6,700	-	2,600
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	50% point																											
Spark	6,700	-	2,600																									
N [%]	6.08																											
$\Omega(\text{CO}_2)$ [%]																												
$T_{\text{phase transition}}$ [°C]	No change in physical form and no loss of hydrate up to 200 °C <sup>[13]</sup>																											
$T_{\text{dec.}}$ [°C]	<p>DSC, exotherm, 0.47–0.52 mg samples<sup>[8]</sup>:</p> <table border="1"> <thead> <tr> <th>Heating rate (K/min)</th><th><math>T_{\text{onset}}</math> (K)</th><th><math>T_{\text{max}}</math> (K)</th></tr> </thead> <tbody> <tr> <td>2.5</td><td>518</td><td>525</td></tr> <tr> <td>5</td><td>525</td><td>533</td></tr> <tr> <td>10</td><td>533</td><td>541</td></tr> <tr> <td>20</td><td>542</td><td>549</td></tr> </tbody> </table> <p>&gt;200 (begins dec.)<sup>[12]</sup></p>	Heating rate (K/min)	$T_{\text{onset}}$ (K)	$T_{\text{max}}$ (K)	2.5	518	525	5	525	533	10	533	541	20	542	549												
Heating rate (K/min)	$T_{\text{onset}}$ (K)	$T_{\text{max}}$ (K)																										
2.5	518	525																										
5	525	533																										
10	533	541																										
20	542	549																										

$\rho$ [g cm <sup>-3</sup> ]	3.878 (yellow needles) <sup>[1]</sup> , 4.059 (red prisms) <sup>[1]</sup> , 1.4–1.6 (apparent density) <sup>[1]</sup> , 3.9 (crystal) <sup>[2]</sup> , sp. gr. ${}^{30}{}^{\circ}\text{C}$ ${}_{30}{}^{\circ}\text{C}$ = 4.05 (orthorhombic yellow-tan crystals) <sup>[7]</sup> , sp. gr. ${}^{30}{}^{\circ}\text{C}$ ${}_{30}{}^{\circ}\text{C}$ = 4.12 (red, diamond-shaped crystals) <sup>[7]</sup> , sp. gr. ${}^{30}{}^{\circ}\text{C}$ ${}_{30}{}^{\circ}\text{C}$ = 4.13 (yellow, amorphous) <sup>[7]</sup> , 1.67 (apparent $\rho$ of dry solid, orthorhombic yellow-tan crystals) <sup>[7]</sup> , 0.59 (apparent $\rho$ of dry solid, red, diamond-shaped crystals) <sup>[7]</sup> , 1.0 (apparent $\rho$ of dry solid, yellow, amorphous) <sup>[7]</sup>		
Heat of formation	$-981.70 \pm 7.11$ kJ/mol ( $\Delta_f H^\circ$ , monobasic LS) <sup>[14]</sup> , $-1,995.99 \pm 7.69$ kJ/mol ( $\Delta_f H^\circ$ , tribasic LS dihydrate) <sup>[14]</sup> , $-2,487.84 \pm 8.61$ kJ/mol ( $\Delta_f H^\circ$ , pentabasic LS dihydrate) <sup>[14]</sup>		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{\text{ex}} U^\circ$ [kJ kg <sup>-1</sup> ]			
$T_{\text{ex}}$ [K]			
$p_{\text{CJ}}$ [kbar]			
VoD [m s <sup>-1</sup> ]			
$V_0$ [L kg <sup>-1</sup> ]			
Sand test [g]	Yellow-tan (orthorhombic) basic LS crushed more sand and shattered the metal cap more completely than red diamond-shaped crystals of LS or yellow amorphous LS <sup>[7]</sup>		
Initiation efficiency	Sensitivity of basic LS in wire bridge initiators, W wire 0.030 in long fired @ 14–20 V <sup>[3]</sup> : 125 Erg for 0.0001 in diameter <sup>[3]</sup> , 700 Erg for 0.00029 in diameter <sup>[3]</sup>		
5 s explosion $T$ [ $^{\circ}\text{C}$ ] Autoignition $T$ [K] Ignition $T$ [ $^{\circ}\text{C}$ ]	508 <sup>[2]</sup>  248–250 <sup>[4]</sup> , 344 (instantaneous, yellow-tan (orthorhombic) basic LS) <sup>[7]</sup> , 240 <sup>[8]</sup> , 250–257 (red-brown granules) <sup>[12]</sup> , 248–250 (oval-shaped yellow-brown crystals) <sup>[12]</sup>		
Thermal stability	No weight loss @ 170 °C for 2 h @ 10 mm Hg <sup>[4]</sup>		
Solubility [g/mL]	Soluble in aq. ammonium acetate <sup>[1]</sup> , practically insoluble in water <sup>[1]</sup> , insoluble in Et <sub>2</sub> O, CHCl <sub>3</sub> , CCl <sub>4</sub> , CS <sub>2</sub> , benzene, toluene, conc. hydrochloric acid and glacial acetic acid <sup>[1]</sup> , slightly soluble in aq. ammonium acetate <sup>[13]</sup>		
Hygroscopicity	No change in explosive properties of yellow-tan (orthorhombic) basic LS after extended storage @ 74 °C and 90% RH <sup>[7]</sup>		

Firing times of hot bridgewire initiators	50 mg loads of explosives, voltage of 450 V, times in $\mu\text{s}^{[3]}$ :			
Milling time (h)	Capacitance ( $\mu\text{F}$ )			
	0.5	0.05	0.0047	
24	10.6–13.1	11.2–23.1	20.0–430.0	
64	4.4–13.0	12.5–14.4	10.6–60.6	
Heat of dec. [J/g]	1,110 (DSC @ 2.5 K/min) <sup>[8]</sup> , 1,200 (DSC @ 5 K/min) <sup>[8]</sup> , 1,180 (DSC @ 10 K/min) <sup>[8]</sup> , 1,190 (DSC @ 20 K/min) <sup>[8]</sup>			

† Three modifications of the  $\beta$ -polymorph of basic LS have been reported (tan-yellow, RD1346-A; red, RD1346 and tan, RD1349) by altering the crystal habit by the addition of 2-nitroresorcinol<sup>[6]</sup>; there is also an  $\alpha$ -polymorph (tan-brown) which is commercially available.<sup>[6]</sup>

	Basic LS <sup>[7]</sup>
Chemical formula	$\text{C}_6\text{H}_3\text{N}_3\text{O}_{10}\text{Pb}_2$
Molecular weight [g mol <sup>-1</sup> ]	
Crystal system	Orthorhombic
Space group	
<i>a</i> [ $\text{\AA}$ ]	8.16 $\pm$ 0.15
<i>b</i> [ $\text{\AA}$ ]	8.24 $\pm$ 0.15
<i>c</i> [ $\text{\AA}$ ]	18.27 $\pm$ 0.30
$\alpha$ [°]	90
$\beta$ [°]	90
$\gamma$ [°]	90
<i>V</i> [ $\text{\AA}^3$ ]	
<i>Z</i>	4
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	
<i>T</i> [K]	
	Yellow-tan

Two crystal forms: yellow needles and red prisms<sup>[1]</sup>. Monobasic LS exists in three polymorphic forms<sup>[4]</sup>; reddish-brown RD1346 shows rounded crystal aggregates with 0.05–0.10 mm particle size<sup>[6]</sup>, crystal shape and size of  $\beta$ -polymorphs depends on the method of preparation.<sup>[6]</sup>

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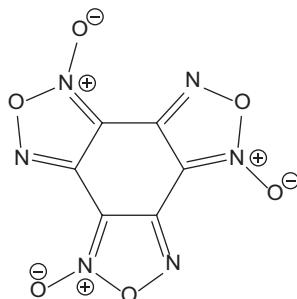
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- [12] G. W. C. Taylor, A. T. Thomas, *Manufacture of Basic Lead Styphnate*, US Patent 3894068, July 8th **1975**.
- [13] G. W. C. Taylor, A. T. Thomas, *Lead Styphnate: Part 4: The Monobasic Lead Salts of Trinitroresorcinol, Polymorphic Modifications and the Development of R.D. 1346 and R.D. 1349*, Report No. 9/R/62, Explosives Research and Development Establishment, Ministry of Aviation, Essex, U.K., 23rd February **1962**.
- [14] J. R. Payne, *Thermochim. Acta*, **1994**, 242, 13–21.
- [15] Z. Shunguan, W. Youchen, Z. Wenyi, M. Jingyan, *Propellants, Explosives, Pyrotechnics*, **1997**, 22, 317–320.

## Benzotrifuroxan

Name [German, acronym]: Benzotrifuroxan, hexanitrosobenzene, benzotriis-[1,2,5]oxadiazole-[4,4,7]-trioxide [benzotrifuroxan, BTF]

Main (potential) use: explosive

Structural formula:



	<b>BTF</b>									
Formula	$C_6N_6O_6$									
Molecular mass [g mol <sup>-1</sup> ]	252.1									
Appearance at RT										
IS [J]	$H_{50} = 11$ cm (tool type 12, 5 kg mass) <sup>[1]</sup> , $H_{50\%} = 53$ cm (B.M., type 12 tool, 2.5 kg mass, 35 mg sample, garnet paper) <sup>[12]</sup> , $H_{50} = 50$ cm <sup>[13]</sup> , $H_{50} = 53$ cm (2.5 kg mass, type 12 tool) <sup>[18]</sup> , $DH_{50} = 94$ cm <sup>[20]</sup> , $A_{d1} = 92\%$ , $A_{d2} = 96\%$ , $LL = 0.5$ m, $A_{50\ d1} = 1.6$ m, $A_{50\ d2} = 1.3$ <sup>[22]</sup> , $H_{50} = 22.7 \pm 0.17$ cm (fine powder, type 12, ERL apparatus) <sup>[27]</sup> , $H_{50} = 45.2 \pm 0.09$ cm (fine powder, type 12, ERL apparatus) <sup>[27]</sup> , $H_{50} = 13.8 \pm 0.05$ cm (blend of needles and powder, type 12, ERL apparatus) <sup>[27]</sup> , $H_{50\%} = 53$ cm (2.5 kg mass, type 12 tool, 35 mg sample in conical pile, 1 in <sup>2</sup> garnet paper) <sup>[29]</sup> , $H_{50\%} = 53$ cm (2.5 kg mass) <sup>[30]</sup>									
FS [N]	$p_{fr,LL} = 150$ MPa <sup>[22]</sup> , $p_{fr,50\%} = 260$ MPa <sup>[22]</sup>									
ESD [J]	Data from <sup>[25]</sup> : <table border="1"> <thead> <tr> <th colspan="3">50% point energy (J)</th> </tr> <tr> <th>3 mil foil</th> <th>10 mil foil</th> <th>% expl.</th> </tr> </thead> <tbody> <tr> <td>0.14</td> <td>0.19</td> <td>85.7</td> </tr> </tbody> </table>	50% point energy (J)			3 mil foil	10 mil foil	% expl.	0.14	0.19	85.7
50% point energy (J)										
3 mil foil	10 mil foil	% expl.								
0.14	0.19	85.7								
N [%]	33.3									
$\Omega(CO_2)$ [%]	-38.1									
$T_{m.p.}$ [°C]	198–200 <sup>[1]</sup> , 195 <sup>[27]</sup>									
$T_{\text{phase transition}}$ [°C]	100–135 <sup>[6]</sup>									

$T_{\text{dec.}} [^{\circ}\text{C}]$	230 (dec. onset) <sup>[14]</sup> $T_{\text{idb}} (\text{@ } 8 \text{ }^{\circ}\text{C}/\text{min}) = 242.9$ ; $T_w (\text{@ } 8 \text{ }^{\circ}\text{C}/\text{min}) = 247.6$ ; $T_{\text{max}} (\text{@ } 8 \text{ }^{\circ}\text{C}/\text{min}) = 255.5$ <sup>[9]</sup> $T_{\text{idb}} (\text{@ } 16 \text{ }^{\circ}\text{C}/\text{min}) = 250.7$ ; $T_w (\text{@ } 16 \text{ }^{\circ}\text{C}/\text{min}) = 266.6$ ; $T_{\text{max}} (\text{@ } 16 \text{ }^{\circ}\text{C}/\text{min}) = 273.4$ <sup>[9]</sup> $T_{\text{cr}} = 248\text{--}251$ <sup>[9]</sup>		
$\rho [\text{g cm}^{-3}]$	1.901 (@ TMD) <sup>[1,2,21]</sup> , 1.87 (nominal) <sup>[1]</sup> , 1.901 <sup>[13,14,27]</sup> , 1.90 <sup>[23,29]</sup> , 1.903 (single crystal) <sup>[24]</sup>		
Heat of formation	144.5 kcal mol <sup>-1</sup> <sup>[1,4]</sup> , 144.9 kcal/mol ( $\Delta H_f$ (s), exptl.) <sup>[13,20]</sup> , 601.7 kJ/mol <sup>[21]</sup> , 2399 kJ/kg <sup>[1]</sup> , 590 kJ/mol (enthalpy of form.) <sup>[14]</sup> , 551.0 kcal/kg (enthalpy of form.) <sup>[15]</sup> , 606 kJ/mol ( $\Delta H_f$ ) <sup>[23]</sup> , 2.31 MJ/kg (enthalpy of form.) <sup>[24]</sup> , 144.0 kcal/mol <sup>[26]</sup> , 143.8 kcal/mol ( $\Delta H_f^o$ ) <sup>[27]</sup> , 144.5 kcal/mol ( $\Delta H_f^o$ ) <sup>[28]</sup>		
Heat of combustion	$-708.1 \text{ kcal mol}^{-1}$ <sup>[4,27]</sup>		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{\text{ex}} U^o [\text{kJ kg}^{-1}]$		169 kcal/g [H <sub>2</sub> O (l)] (calcd. using rxn. enthalpies) <sup>[1]</sup>  169 kcal/g [H <sub>2</sub> O (g)] (calcd. using rxn. enthalpies) <sup>[1]</sup>  1.41 kcal/g [H <sub>2</sub> O (l)] <sup>[7]</sup>  1.69 kcal/g ( $Q_{\text{max}}$ , calcd.) <sup>[13]</sup>  5,860 <sup>[14]</sup>  1,162 kcal/kg (@ 0.950 g cm <sup>-3</sup> , calcd.) [H <sub>2</sub> O vapor] <sup>[15]</sup>  $-\Delta H_{\text{det}} = 7.07 \text{ kJ/g}$ <sup>[23]</sup>	141 kcal/g [H <sub>2</sub> O (l)] <sup>[1]</sup>  141 kcal/g [H <sub>2</sub> O (g)] <sup>[1]</sup>  1160 kcal/kg (@ 0.950 g cm <sup>-3</sup> ) [H <sub>2</sub> O vapor] <sup>[15]</sup>  5.80 MJ/kg (@ 1.82 g cm <sup>-3</sup> ) <sup>[24]</sup>  5.90 MJ/kg (@ 1.86 g cm <sup>-3</sup> ) <sup>[24]</sup>
$T_{\text{ex}} [\text{K}]$		4,590 (@ 1.86 g cm <sup>-3</sup> , calcd. BKWR) <sup>[26]</sup>  5,570 (@ 1.86 g cm <sup>-3</sup> , calcd. BKWS) <sup>[26]</sup>	3,990 (@ 1.82 g cm <sup>-3</sup> ) <sup>[24]</sup>  4,170 (@ 1.84 g cm <sup>-3</sup> ) <sup>[24]</sup>

		4,700 (@ 1.76 g cm <sup>-3</sup> , calcd. BKWR) <sup>[26]</sup>  5,600 (@ 1.76 g cm <sup>-3</sup> , calcd. BKWS) <sup>[26]</sup>	
$p_{C_J}$ [kbar]		331 (calcd., K-J) <sup>[4]</sup> 294 (calcd. Ruby code) <sup>[1]</sup> 358 (@ 1.859 g cm <sup>-3</sup> , calcd. empirical) <sup>[10]</sup> ~360 <sup>[7]</sup> 331 (@ 1.901 g cm <sup>-3</sup> , calcd.) <sup>[13]</sup> 343 (@ 1.86 g cm <sup>-3</sup> , calcd. BKWR) <sup>[26]</sup> 336 (@ 1.86 g cm <sup>-3</sup> , calcd. BKWS) <sup>[26]</sup> 307 (@ 1.76 g cm <sup>-3</sup> , calcd. BKWR) <sup>[26]</sup> 302 (@ 1.76 g cm <sup>-3</sup> , calcd. BKWS) <sup>[26]</sup> 330 (@ 2.12 g cm <sup>-3</sup> , calcd.) <sup>[29]</sup>	0.360 Mbar (est.) <sup>[1]</sup> 34.6 GPa <sup>[8]</sup> 360 (@ 1.850 g cm <sup>-3</sup> ) <sup>[10]</sup> 30.5 GPa <sup>[20]</sup> 33.0–36.0 GPa (@ 1.85–1.86 g cm <sup>-3</sup> ) <sup>[24]</sup> 33.8 GPa (@ 1.82 g cm <sup>-3</sup> ) <sup>[24]</sup> 34.5 GPa (@ 1.84 g cm <sup>-3</sup> ) <sup>[24]</sup> 360 (@ 1.86 g cm <sup>-3</sup> ) <sup>[26]</sup>
VoD [m s <sup>-1</sup> ]		8,500 (@ 1.90 g cm <sup>-3</sup> , calcd. K-J) <sup>[4]</sup> 8,531 (@ 1.859 g cm <sup>-3</sup> , calcd., empirical) <sup>[10]</sup> 8,500 (@ 1.901 g cm <sup>-3</sup> , calcd.) <sup>[13]</sup> 8,430 (@ 1.86 g cm <sup>-3</sup> , calcd. BKWR) <sup>[26]</sup> 8,400 (@ 1.86 g cm <sup>-3</sup> , calcd. BKWS) <sup>[26]</sup> 8,140 (@ 1.76 g cm <sup>-3</sup> , calcd. BKWR) <sup>[26]</sup>	8,485 (@ 1.859 g cm <sup>-3</sup> ) <sup>[1,5]</sup> 8,260 (@ 1.901 g cm <sup>-3</sup> ) <sup>[4]</sup> 8,260 (@ 1.76 g cm <sup>-3</sup> ) <sup>[8,26]</sup> 8,260 (@ 1.90 g cm <sup>-3</sup> ) <sup>[8]</sup> 7,990 (@ 1.88 g cm <sup>-3</sup> ) <sup>[8]</sup> 8,485 (@ 1.859 g cm <sup>-3</sup> ) <sup>[10]</sup> 8,490 (@ 1.86 g cm <sup>-3</sup> ) <sup>[11,26]</sup> 8,490 (@ 1.85–1.86 g cm <sup>-3</sup> ) <sup>[24]</sup>

		8,140 (@ 1.76 g cm <sup>-3</sup> , calcd. BKWS) <sup>[26]</sup>  8,420 (@ 2.12 g cm <sup>-3</sup> , calcd.) <sup>[29]</sup>																																												
$V_0$ [L kg <sup>-1</sup> ]																																														
$I_{sp}$ [Ns g <sup>-1</sup> ]		2.65 (calcd., ISPBKW code) <sup>[28]</sup> , 2.53 (calcd., empirical) <sup>[28]</sup>																																												
Critical diameter [cm]		$d_{c0}$ (mm) @ mean crystal size ( $\mu\text{m}$ ) <sup>[14]</sup> : 0.06 @ 3, 0.15 @ 10, 0.30 @ 20 <sup>[14]</sup> , failure diameter = 0.5–1.0 mm <sup>[24]</sup>																																												
Critical temperature [°C]		248–251 (exptl.) <sup>[16,19]</sup> , 275 (calcd.) <sup>[16,19]</sup> , 249 ± 1 ( $T_m$ ) <sup>[27]</sup>																																												
LLNL reactivity test		0.05 cm <sup>3</sup> gas evolved per 0.25 g sample @ 120 °C for 22 h <sup>[1]</sup>																																												
Cylinder velocities		Values from ref <sup>[17]</sup> , $\theta = 1.80$ g cm <sup>-3</sup> , Cu cylinder, $R$ = current value of outer radius of cylinder, $R_0$ = initial value of outer radius of cylinder <sup>[17]</sup> :	<table border="1"> <thead> <tr> <th></th> <th colspan="6"><math>R - R_0</math> (mm)</th> </tr> <tr> <th>Exptl.</th> <th>1.51</th> <th>1.58</th> <th>1.65</th> <th>1.71</th> <th>1.75</th> <th>1.79</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>1.49</td> <td>1.55</td> <td>1.63</td> <td>1.69</td> <td>1.72</td> <td>1.76</td> </tr> <tr> <td>2</td> <td>1.49</td> <td>1.55</td> <td>1.63</td> <td>1.69</td> <td>1.72</td> <td>1.76</td> </tr> </tbody> </table> <p>Summary of experimental copper cylinder wall velocity data, PETN with a density of 1.763 g/cm<sup>3</sup> is the reference explosive, data from<sup>[21]</sup>:</p> <table border="1"> <thead> <tr> <th>Initial density (g/cm<sup>3</sup>)</th> <th>Inner diameter (mm)</th> <th>Wall thickness (mm)</th> <th>Wall velocity (mm/μs) at 25.4 mm diameter for <math>R - R_0</math> equal to</th> <th>Velocity-squared cf. with PETN for the same configuration, % comparison <math>R - R_0</math> equal to</th> </tr> </thead> <tbody> <tr> <td></td> <td></td> <td></td> <td>6 mm    12.5 mm    19 mm</td> <td>6 mm    12.5 mm    19 mm</td> </tr> <tr> <td>1.852</td> <td>25.44</td> <td>2.601</td> <td>1.605    1.755    1.835</td> <td>5.9    6.0    5.1</td> </tr> </tbody> </table>		$R - R_0$ (mm)						Exptl.	1.51	1.58	1.65	1.71	1.75	1.79	1	1.49	1.55	1.63	1.69	1.72	1.76	2	1.49	1.55	1.63	1.69	1.72	1.76	Initial density (g/cm <sup>3</sup> )	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	1.852	25.44	2.601	1.605    1.755    1.835	5.9    6.0    5.1
	$R - R_0$ (mm)																																													
Exptl.	1.51	1.58	1.65	1.71	1.75	1.79																																								
1	1.49	1.55	1.63	1.69	1.72	1.76																																								
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Initial density (g/cm <sup>3</sup> )	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																																										
1.852	25.44	2.601	1.605    1.755    1.835	5.9    6.0    5.1																																										
Heat of dec. [cal/g]		600 ( $Q$ , heat of dec. reaction) <sup>[27]</sup>																																												
Plate dent test		Dent depth = 3.05 mm @ 1.838 g cm <sup>-3</sup> (12.7 mm explosive diameter) <sup>[27]</sup>																																												

Summary of code calculations with measured detonation velocities and detonation energies derived from JWL's<sup>[21]</sup>:

Initial density (g/cm <sup>3</sup> )	PETN-adjusted BKWR Tiger, LLNL library, $\theta = 1850$ 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
1.852	-2	-3	-3	10	4	2	2	-1	-1

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 at 298 K. Code-calculated energies with the 1,800 K freeze are also included, data from<sup>[21]</sup>:

Measured density (g/cm <sup>3</sup> )	Measured confined heat of detonation (kJ/cm <sup>3</sup> )	Density from <sup>[87]</sup>	Heat of detonation using density from <sup>[87]</sup>	Energy of detonation, $E_0$ (kJ/cm <sup>3</sup> )			
				From heat of detonation	Freeze at 1,800 K		
					Tiger BKWR	Tiger JCZ3	CHEQ
1.86	-10.98	1.852	-10.93	-11.2	-10.7	-10.2	-11.0

JWL cylinder coefficient data from<sup>[21]</sup>:

Initial density, $\rho_0$ (g/cm <sup>3</sup> )	Detonation velocity, $D$ (mm/μs)	Energy of detonation, $E_0$ (kJ/cm <sup>3</sup> )	CJ pressure (GPa)	A (GPa)	B (GPa)	C (GPa)	$R_1$	$R_2$	$\omega$	$\gamma_{\text{CJ}}$
1.852	8.49	-11.30	34.0	945.6163	22.66797	2.956620	5.027	1.60	0.50	2.926

	<b>BTF<sup>[6]</sup></b>	<b>BTF<sup>[1,2,3]</sup></b>	<b>BTF</b> (freshly prepared crystals) <sup>[6]</sup>	<b>BTF</b> (stored 6 months @ 5 °C) <sup>[6]</sup>	<b>BTF</b> (stored 6 months @ 20 °C) <sup>[6]</sup>	<b>BTF</b> (warming 12 h @ 80 °C) <sup>[6]</sup>	<b>BTF</b> (warming 2 h @ 120 °C) <sup>[6]</sup>
Chemical formula	C <sub>6</sub> N <sub>6</sub> O <sub>6</sub>	C <sub>6</sub> N <sub>6</sub> O <sub>6</sub>	C <sub>6</sub> N <sub>6</sub> O <sub>6</sub>	C <sub>6</sub> N <sub>6</sub> O <sub>6</sub>	C <sub>6</sub> N <sub>6</sub> O <sub>6</sub>	C <sub>6</sub> N <sub>6</sub> O <sub>6</sub>	C <sub>6</sub> N <sub>6</sub> O <sub>6</sub>
Molecular weight [g mol <sup>-1</sup> ]	252.1	252.1	252.1	252.1	252.1	252.1	252.1
Crystal system	Orthorhombic	Orthorhombic	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	Pna2 <sub>1</sub> (no. 33)	Pna2 <sub>1</sub> (no. 33)	P2 <sub>1</sub> /a (no. 14)	P2 <sub>1</sub> /a (no. 14)	P2 <sub>1</sub> /a (no. 14)	P2 <sub>1</sub> /a (no. 14)	P2 <sub>1</sub> /a (no. 14)
<i>a</i> [Å]	6.923(1) ± 0.0009	6.9234 ± 0.0009	14.661	14.750	14.969	15.055	15.082
<i>b</i> [Å]	19.516(3) ± 0.0012	19.5158 ± 0.0012	10.219	10.226	10.209	10.168	10.168
<i>c</i> [Å]	6.518(1) ± 0.0013	6.5180 ± 0.0012	12.032	11.914	11.816	11.714	11.735
α [°]	90	90	90	90	90	90	90
β [°]	90	90	90	90	90	90	90
γ [°]	90	90	103.72	103.40	102.44	102.20	102.20
<i>V</i> [Å <sup>3</sup> ]	880.642	Not specified	1,751.21	1,748.1	1,763.3	1,752.8	1,759.0
<i>Z</i>	4	4	8	8	8	8	8
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.901	1.901	1.912	1.915	1.898	1.910	1.903
<i>T</i> [K]	295	298	295	295	295	295	295

Freshly prepared monoclinic BTF shows two crystallographically independent molecules with conformation M; after 6 months storage at RT different conformations (M and P) present<sup>[6]</sup>. BTF crystals after heating @ 120 °C for 2 h: P and N conformations in unit cell. N is an intermediate conformation in transition of isomers M–P<sup>[6]</sup>. Therefore, essentially three phases: (i) monoclinic  $P2_1/a$  (A) with M and M conformations, (ii) monoclinic  $P2_1/a$  (A) with M and P conformations, (iii) monoclinic  $P2_1/a$  (A) with P and N conformations, and also (iv) orthorhombic  $Pna2_1$  (B).<sup>[6]</sup>

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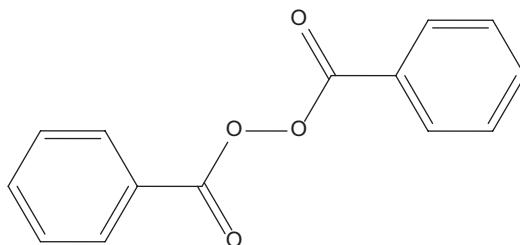
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## Benzoyl peroxide

Name [German, acronym]: Benzoyl peroxide, dibenzoyl peroxide, benzoyl superoxide, benoxyl, Oxy-5, persadox, lucidol  
[Benzoylperoxid, BPO]

Main (potential) use: Catalyst for polymerization reactions<sup>[1]</sup>

Structural formula:



	<b>Benzoyl peroxide</b>
Formula	C <sub>14</sub> H <sub>10</sub> O <sub>4</sub>
Molecular mass [g mol <sup>-1</sup> ]	242.23
Appearance at RT	White crystals or powder <sup>[10]</sup> , crystals <sup>[19]</sup>
IS [J]	5 <sup>[1]</sup> , h = 10 cm (sandpaper, NOL/ERL apparatus, 98.5% benzoyl peroxide (dry)) <sup>[7]</sup> , 4 in (2 kg mass, 16 mg sample P.A. apparatus) <sup>[8]</sup> , h = 19 cm (NOL/ERL apparatus, bone tools) <sup>[7]</sup>
FS [N]	240 <sup>[1]</sup> , 120 N pistil load <sup>[1]</sup>
N [%]	0
Ω(CO <sub>2</sub> ) [%]	-191.6
T <sub>m.p.</sub> [°C]	103–106 <sup>[2,19]</sup> , 103.5 <sup>[9]</sup> , 104–106 (dec.) <sup>[8]</sup> , 103–105 (dec.) <sup>[10]</sup> , 105 <sup>[22]</sup>
T <sub>dec.</sub> [°C]	107 <sup>[3]</sup> , 108 <sup>[5]</sup> , 91 (onset, DSC @ 28 °C/min) <sup>[5,6]</sup> , 96 (DSC @ 15 °C/min) <sup>[5]</sup> , 103–105 <sup>[10]</sup> , may explode when heated <sup>[19]</sup>
ρ [g cm <sup>-3</sup> ]	1.334 (@ 298.15 K) <sup>[2]</sup> , 1.34 (crystal @ 298 K) <sup>[9]</sup> , 1.33 (measured) <sup>[9]</sup> , 1.3 <sup>[10]</sup>
Heat of formation	-382.5 kJ/mol (enthalpy of form., calcd., emp.) <sup>[4]</sup> , -369 kJ/mol (enthalpy of form., exptl.) <sup>[4]</sup> , -183.8 kJ/mol (enthalpy of form., calcd., S-D method) <sup>[4]</sup> , -392.5 kJ/mol <sup>[11,12]</sup> , -393.0 ± 6.3 kJ/mol (s) <sup>[11,12]</sup> , -369.0 ± 4.6 kJ/mol (s) <sup>[11,12]</sup> , -369.0 ± 8.4 kJ/mol (s) <sup>[11,12]</sup> , -272.0 ± 5.4 kJ/mol (g) <sup>[11,12]</sup> , -281.7 ± 6.2 kJ/mol (g) <sup>[11,12]</sup>

Heat of combustion [kJ/mol]	$Q_c^V = 1,552 \text{ kcal/mol}^{[8]}, 6,417 \text{ cal/g}^{[8]}$		
	Calcd. (EXPLO5 6.03)	Lit. values	exptl.
$-\Delta_{\text{ex}}U^\circ [\text{kJ kg}^{-1}]$	1,556	2.37 MJ/kg (calcd., SD code) <sup>[13]</sup>	
$T_{\text{ex}} [\text{K}]$	1,336	1,609 (calcd., SD code) <sup>[13]</sup>	
$p_{\text{CJ}} [\text{kbar}]$	48.1	1.89 GPa (calcd., SD code) <sup>[13]</sup>	
VoD [ $\text{m s}^{-1}$ ]	4,272 (@ TMD)	2,960 (@ 1.1 g $\text{cm}^{-3}$ , calcd., SD code) <sup>[13]</sup>	1,280–700 (@ 0.4 g $\text{cm}^{-3}$ , steel tube, 240 mm length, powerful initiation) <sup>[6]</sup>  800 (@ 0.57 g $\text{cm}^{-3}$ , steel tube, 240 mm length, cap no. 8 initiation) <sup>[6]</sup>
$V_0 [\text{L kg}^{-1}]$	449		

Trauzl test [cm <sup>3</sup> , % TNT]	28.0 (Trauzl test number, 99% benzoyl peroxide, 6.0 g sample, 3 dram vial with plastic cap with opening for no. 8 blasting cap) <sup>[17]</sup> , 9.0 (Trauzl test number, 70% benzoyl peroxide, wet, 6.0 g sample, 3 dram vial with plastic cap with opening for no. 8 blasting cap) <sup>[17]</sup> , 31 ml / 10 g <sup>[18]</sup> , 21 ml / 10 g (75% benzoyl peroxide with water) <sup>[18]</sup>																																																																						
Sand test [g]	5.2 g sand crushed <sup>[8]</sup>																																																																						
Ballistic mortar test	<p>15.5% TNT (weight strength)<sup>[14]</sup></p> <p>Using the MkIIIF mortar, length of swing (<math>d</math>) together with the weight of PETN booster (<math>W_{\text{PETN}}</math>)<sup>[15]</sup>:</p> <table border="1"> <thead> <tr> <th rowspan="2">Material</th> <th colspan="5">Length of swing (mm), accurate weight of PETN given in 0 in g</th> </tr> <tr> <th>5 g</th> <th>8 g</th> <th>10 g</th> <th>15 g</th> <th>20 g</th> </tr> </thead> <tbody> <tr> <td>BPO, 8 g (no projectile)</td> <td>32 (0.0)</td> <td>33 (0.1107)</td> <td>35 (0.2175)</td> <td>39 (0.4259)</td> <td>41 (0.5212)</td> </tr> <tr> <td>BPO, 8 g (2.0 kg projectile)</td> <td>105 (0.0)</td> <td>110 (0.1107)</td> <td>111 (0.2124)</td> <td>119 (0.4008)</td> <td>126 (0.6105)</td> </tr> <tr> <td>BPO 75% with H<sub>2</sub>O, 10 g</td> <td>49 (0.0)</td> <td>84 (0.1056)</td> <td>82 (0.2055)</td> <td>92 (0.3299)</td> <td>123 (0.4001)</td> </tr> <tr> <td></td> <td></td> <td></td> <td></td> <td>134 (0.5015)</td> <td>136 (0.6069)</td> </tr> </tbody> </table> <p>Length of swing (<math>d</math>) together with the weight of organic peroxide (<math>W_s</math>)<sup>[15]</sup>:</p> <table border="1"> <thead> <tr> <th rowspan="2">Material</th> <th colspan="5">Length of swing (mm), accurate weight of PETN given in () in g</th> </tr> <tr> <th>5 g</th> <th>8 g</th> <th>10 g</th> <th>15 g</th> <th>20 g</th> </tr> </thead> <tbody> <tr> <td>BPO (2 kg projectile)</td> <td>97 (0.06014)</td> <td>119 (0.6008)</td> <td>148 (0.6038)</td> <td>175 (0.6042)</td> <td>211 (0.6258)</td> </tr> <tr> <td>BPO (no projectile)</td> <td>30 (0.6068)</td> <td>49 (0.6210)</td> <td>64 (0.6134)</td> <td>82 (0.6220)</td> <td>99 (0.6109)</td> </tr> <tr> <td>BPO 75% with H<sub>2</sub>O (2 kg projectile)</td> <td>106 (0.6232)</td> <td>136 (0.6062)</td> <td>142 (0.6275)</td> <td>136 (0.6168)</td> <td>131 (0.6195)</td> </tr> <tr> <td></td> <td></td> <td></td> <td></td> <td>166 (0.6095)</td> <td>118 (0.6149)</td> </tr> </tbody> </table>	Material	Length of swing (mm), accurate weight of PETN given in 0 in g					5 g	8 g	10 g	15 g	20 g	BPO, 8 g (no projectile)	32 (0.0)	33 (0.1107)	35 (0.2175)	39 (0.4259)	41 (0.5212)	BPO, 8 g (2.0 kg projectile)	105 (0.0)	110 (0.1107)	111 (0.2124)	119 (0.4008)	126 (0.6105)	BPO 75% with H <sub>2</sub> O, 10 g	49 (0.0)	84 (0.1056)	82 (0.2055)	92 (0.3299)	123 (0.4001)					134 (0.5015)	136 (0.6069)	Material	Length of swing (mm), accurate weight of PETN given in () in g					5 g	8 g	10 g	15 g	20 g	BPO (2 kg projectile)	97 (0.06014)	119 (0.6008)	148 (0.6038)	175 (0.6042)	211 (0.6258)	BPO (no projectile)	30 (0.6068)	49 (0.6210)	64 (0.6134)	82 (0.6220)	99 (0.6109)	BPO 75% with H <sub>2</sub> O (2 kg projectile)	106 (0.6232)	136 (0.6062)	142 (0.6275)	136 (0.6168)	131 (0.6195)					166 (0.6095)	118 (0.6149)
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Shock sensitivity	BPO: shock sensitivity = high, complete explosion with a no. 0 detonator, propagation of explosion = yes, explosive power = 25% TNT <sup>[15]</sup>
	BPO 75% with H <sub>2</sub> O: shock sensitivity = no, propagation of explosion = no, explosive power = no <sup>[15]</sup>
Underwater energy release tests	Rel. bubble energies (rel. energy/unit mass) = 42.7% TNT <sup>[14]</sup> , rel. bubble energy = 28.8% for wet BPO (with 22% H <sub>2</sub> O) <sup>[14]</sup>
Card gap test	Sample contained in 40 cm long, cold-drawn seamless mechanical tube, outside diameter = 4.76 cm, wall thickness = 0.55 cm, cast pentolite booster of 5.0 cm diameter and 5.00 cm long weighing ~175 g used to initiate charge, test carried out at 20 °C ± 1 °C, loading $\rho = 0.46 \text{ g cm}^{-3}$ , BPO not shock sensitive since no damage to witness plate, shock wave decays to 950 m/s in each test <sup>[14]</sup> .
Deflagration-to-detonation transition test	Sample loaded in non vented bomb of 45.7 cm length, schedule 80 steel pipe capped at both ends with forged steel pipe caps, 7.37 cm inside diameter, 0.76 cm wall thickness, test carried out at 20 °C ± 1 °C <sup>[14]</sup> ; no. of fragments = 0, sample burned, pipe was slightly distorted

Koenen and Ide BAM test	Steel case, interior diameter = 2.4 cm, 7.5 cm long, 0.05 cm wall thickness <sup>[14]</sup> :				
	Orifice diameter, $d$ (mm)	$t_1$ (s)	$t_2$ (s)	Time function $\sqrt{t_1/d + t_2/d}$	Remarks
	8.0	3.5	Instantaneous explosion	0.64	Steel case broke into three pieces
Thermal explosion test					
Sample (loading $\rho = \sim 0.46 \text{ g cm}^{-3}$ ) loaded into schedule 80 steel pipe, 40 cm long, 3.17 cm exterior diameter, non vented pipe closed by schedule 80 caps; explosion $T = 100^\circ\text{C}$ , nonpipe damage <sup>[14]</sup>					
Heavy confinement cap test					
4.0 g sample in 2.0 cm outer diameter glass test tube, length = 7.5 cm, test tube placed in 2.54 cm diameter by 10.8 cm deep hole drilled in a 12.7 cm diameter by 15.0 cm high steel borehole block, no. 8 detonator used; average height = 4.6m, rel. height = 19.2 % Nm, rel. height = 20.1% TNT <sup>[14]</sup>					
5 s explosion $T$ [ $^\circ\text{C}$ ]					
Autoignition $T$ [ $^\circ\text{C}$ ]	80 <sup>[10]</sup>				
Vapor pressure [atm. @ $^\circ\text{C}$ ]		<0.1 kPa @ $20^\circ\text{C}$ <sup>[10,11]</sup>			
Solubility [g/mL]		Poor in $\text{H}_2\text{O}$ <sup>[10]</sup> , sparingly soluble in water, $\text{EtOH}$ <sup>[19]</sup> , soluble in benzene, $\text{CHCl}_3$ , $\text{Et}_2\text{O}$ <sup>[19]</sup> , 1 g dissolves in 40 mL $\text{CS}_2$ <sup>[19]</sup> ,			
1 g dissolves in ~50 mL olive oil <sup>[19]</sup> , solubility in water = 1.550E-04 g/L @ RT <sup>[22]</sup>					
2" steel tube test (UN A1)	Yes <sup>[18]</sup> , no (75% dibenzoyl peroxide with water) <sup>[18]</sup>				

Evaluation of the deflagration hazards of BPO by the revised time–pressure test (5 g sample, igniter =  $\text{Pb}_3\text{O}_4$  (70 wt.%)–Si (30 wt.%), firing method = firing with a nichrome wire or a fusehead, rupture disk = brass, 0.15 mm thickness)<sup>[16]</sup>:

Peroxide	Purity (wt.%)	Active oxygen (wt.%)	Physical appearance	Deflagration properties		
				Amount of igniter (g) <sup>†</sup>	$\Delta t$ (ms)	
					100–300 psi	300–500 psi
BPO	99.9	6.61	Powder	1	0.33	0.15

<sup>†</sup> Giving the apparent max. rate of pressure rise.

Effects of firing methods on the deflagration hazards of BPO by the revised time-pressure test (5 g sample, igniter =  $\text{Pb}_3\text{O}_4$  (70% wt.)–Si (30% wt.), firing method = nichrome, firing with the nichrome wire from the lower side; priming = firing with the fusehead in the center of the samples, rupture disk = brass, 0.15 mm thickness)<sup>[16]</sup>:

Peroxide (active oxygen (wt.%)	Firing method	Igniter			
		1 g $\Delta t$ (ms)		3 g $\Delta t$ (ms)	
		100–300 psi	300–500 psi	100–300 psi	300–500 psi
BPO (6.61)	Nichrome	$3.3 \times 10^{-1}$	$1.5 \times 10^{-1}$	$4.2 \times 10^{-1}$	$1.4 \times 10^{-1}$
BPO (6.61)	Priming	$4.0 \times 10^{-1}$	$1.9 \times 10^{-1}$	$3.6 \times 10^{-1}$	$1.4 \times 10^{-1}$

	Benzoyl peroxide	Benzoyl peroxide <sup>[9]</sup>	Benzoyl peroxide <sup>[20]</sup>	Benzoyl peroxide <sup>[21]</sup>
Chemical formula	$\text{C}_{14}\text{H}_{10}\text{O}_4$	$\text{C}_{14}\text{H}_{10}\text{O}_4$	$\text{C}_{14}\text{H}_{10}\text{O}_4$	$\text{C}_{14}\text{H}_{10}\text{O}_4$
Molecular weight [g mol <sup>-1</sup> ]	242.23	242.23	242.23	242.22
Crystal system	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic
Space group	$P 2_12_12_1$ (no. 19)			
$a$ [\AA]	$8.95 \pm 0.01$	8.950(10)	8.992(2)	8.7959(3)
$b$ [\AA]	$14.24 \pm 0.01$	14.240(10)	14.322(3)	9.1638(4)
$c$ [\AA]	$9.40 \pm 0.02$	9.400(20)	9.446(2)	14.2044(5)
$\alpha$ [°]	90	90	90	90
$\beta$ [°]	90	90	90	90
$\gamma$ [°]	90	90	90	90

$V [\text{\AA}^3]$	1,210	1,198.01	1,216.49	1,144.93(8)
Z	4	4	4	4
$\rho_{\text{calc}} [\text{g cm}^{-3}]$	1.34 ( $D_m = 1.33$ )	1.343	1.32258	1.405
T [K]	298	295	295	100

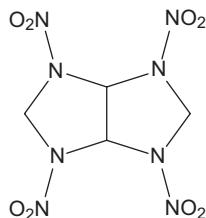
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# Bicyclo-HMX

Name [German, acronym]: 2,4,6,8-Tetranitro-2,4,6,8-tetraazabicyclo[3.3.0] octane,  
[*cis*-1,3,4,6-tetranitrooctahydroimidazo-[4,5-*d*]imidazole],  
*cis*-2,4,6,8-Tetranitro-1*H*,5*H*-2,4,6, 8-tetraazabicyclo[3.3.0]octane  
[bicyclo-HMX, BCHMX]

Main (potential) use: high explosive

Structural formula:



BCHMX			
Formula	$\text{C}_4\text{H}_6\text{N}_8\text{O}_8$		
Molecular mass [g mol <sup>-1</sup> ]	294.14		
Appearance at RT	Colorless rectangular prisms <sup>[5]</sup>		
IS [J]	3 <sup>[6,7]</sup>		
FS [N]	88 <sup>[6,7]</sup>		
ESD [J]	0.150 <sup>[6,7]</sup>		
N [%]	38.10		
$\Omega(\text{CO}_2)$ [%]	-16.3		
$T_{\text{m.p.}}$ [°C]	243–246 (with dec.) <sup>[3]</sup> , 268 <sup>[4]</sup>		
$T_{\text{dec.}}$ [°C]	207 (onset) 220 (extensive dec.) (TG-DTA, 100 mg sample, @ 5 °C/min) <sup>[3]</sup>		
$\rho$ [g cm <sup>-3</sup> ]	1.87 <sup>[1]</sup> , 1.92 <sup>[2]</sup> , 1.86 (predicted TMD) <sup>[4]</sup>		
Heat of formation	125 kJ/mol (enthalpy of form.) <sup>[1]</sup> , 206.3 kJ/mol ( $\Delta_f H^\circ$ , exptl.) <sup>[2]</sup>		
	Calcd. (EXPLO 5 6.04)	Lit. values	Exptl.

$-\Delta_{\text{ex}}U^{\circ} [\text{kJ kg}^{-1}]$		5.758 MJ/kg (heat of explosion) <sup>[4]</sup> 6.518 MJ/kg (calcd. max. heat of explosion) <sup>[4]</sup>	
$T_{\text{ex}} [\text{K}]$			
$p_{\text{CJ}} [\text{kbar}]$		370 (@ 1.86 g cm <sup>-3</sup> , calcd.) <sup>[4]</sup>	
$\text{VoD} [\text{m s}^{-1}]$		9,050 (@ 1.86 g cm <sup>-3</sup> , calcd.) <sup>[4]</sup>	
$V_0 [\text{L kg}^{-1}]$			
5 s explosion $T$ [°C] Ignition $T$ [°C]		214–224 <sup>[4]</sup>	
Burn rate [mm/s]		Burn rate characteristics: pressure interval = 0.02–0.11, pressure exponent = 0.354, burning rate @ 10 MPa = 27.9 mm/s, strand $\rho = 1.82 \text{ g cm}^{-3}$ , adiabatic flame $T$ @ 10 MPa = 3,530 K <sup>[2]</sup>	

	Bicyclo-HMX <sup>[5]</sup>
Chemical formula	C <sub>4</sub> H <sub>6</sub> N <sub>8</sub> O <sub>8</sub>
Molecular weight [g mol <sup>-1</sup> ]	294.17
Crystal system	Monoclinic
Space group	P2 <sub>1</sub>
$a$ [Å]	8.5979(2)
$b$ [Å]	6.9495(2)
$c$ [Å]	8.9726(2)
$\alpha$ [°]	90
$\beta$ [°]	101.783(2)
$\gamma$ [°]	90
$V$ [Å <sup>3</sup> ]	524.83
$Z$	2
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.861
$T$ [K]	294

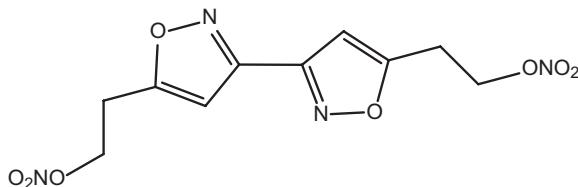
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**[3,3'-Biisoxazole]-5,5'-diylbis(ethane-2,1-diyl)dinitrate**

Name [German, acronym]: [3,3'-Biisoxazole]-5,5'-diylbis(ethane-2,1-diyl)dinitrate,  
 [[3,3'-biisoxazol]-5,5'-diylbis(ethan-2,1-diyl)dinitrat,  
 BIDNE]

Main (potential) use: melt-cast

Structural formula:



<b>BIDNE</b>			
Formula	C <sub>10</sub> H <sub>10</sub> N <sub>4</sub> O <sub>8</sub>		
Molecular mass [g mol <sup>-1</sup> ]	314.21		
Appearance at RT	White powder <sup>[1]</sup>		
IS [J]	>36 (modified P.A. apparatus) <sup>[1]</sup>		
FS [N]	>350 (BAM) <sup>[1]</sup>		
ESD [J]	3.125 (firing test system model 931) <sup>[1]</sup>		
N [%]	17.83		
Ω(CO <sub>2</sub> ) [%]	-35.6		
T <sub>m.p.</sub> [°C]	76.3 <sup>[1]</sup>		
T <sub>dec.</sub> [°C]	200.5 <sup>[1]</sup>		
ρ [g cm <sup>-3</sup> ]	1.565 (X-ray) <sup>[1]</sup>		
Heat of formation	-56.2 kJ/mol (Δ <sub>r</sub> H°, calcd.) <sup>[1]</sup>		
	Calcd. (EXPL05 6.04)	Lit. values	Exptl.
-Δ <sub>ex</sub> U° [kJ kg <sup>-1</sup> ]			
T <sub>ex</sub> [K]			
p <sub>C-J</sub> [kbar]		17.0 GPa (calcd.) <sup>[1]</sup>	
V <sub>oD</sub> [m s <sup>-1</sup> ]		6,910 (@ 1.565 g cm <sup>-3</sup> , calcd.) <sup>[1]</sup>	
V <sub>o</sub> [L kg <sup>-1</sup> ]			

$I_{\text{sp}}$ [s]	200.8 (calcd.) <sup>[1]</sup>
Compatibility	Hydrolytically stable <sup>[1]</sup>

	<b>BIDNE<sup>[1]</sup></b>
Chemical formula	$\text{C}_{10}\text{H}_{10}\text{N}_4\text{O}_8$
Molecular weight [g mol <sup>-1</sup> ]	314.21
Crystal system	Triclinic
Space group	<i>P</i> -1
<i>a</i> [\AA]	4.9591
<i>b</i> [\AA]	7.1150(7)
<i>c</i> [\AA]	10.9653(5)
$\alpha$ [°]	98.072(13)
$\beta$ [°]	76.586(10)
$\gamma$ [°]	88.102(10)
<i>V</i> [\AA <sup>3</sup> ]	333.47(7)
<i>Z</i>	1
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.565
<i>T</i> [K]	296

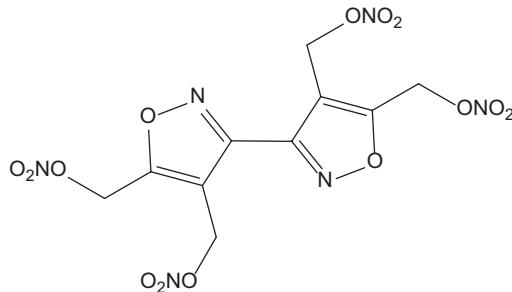
[1] L. A. Wingard, R. C. Sausa, P. E. Guzmán, R. Pesce-Rodriguez, J. J. Sabatini, G. W. Drake, *Propellants, Explosives, Pyrotechnics*, **2019**, *in press*.

## Biisoxazolotetrakis(methyl)nitrate

Name [German, acronym]: Biisoxazolotetrakis(methyl)nitrate, ((3,3'-bi-1,2-oxazole)-4,4',5,5'-(tetrayl)tetrakis(methylene) tetranitrate [BITN]

Main (potential) use: Potential new nitrate plasticizer and possible new ingredient in pyrotechnic percussion primer compositions<sup>[1]</sup>

Structural formula:



	BITN		
Formula	C <sub>10</sub> H <sub>8</sub> N <sub>6</sub> O <sub>14</sub>		
Molecular mass [g mol <sup>-1</sup> ]	436.22		
Appearance at RT			
IS [J]	30 (modified P.A. apparatus) <sup>[1]</sup>		
FS [N]	60 (BAM) <sup>[1]</sup>		
ESD [J]	0.0625 (ABL machine) <sup>[1]</sup>		
N [%]	19.27		
Ω(CO <sub>2</sub> ) [%]	-36.7		
T <sub>m.p.</sub> [°C]	121.9 (onset), 125.0 (peak) (DSC @ 5 °C/min) <sup>[1]</sup>		
T <sub>dec.</sub> [°C]	193.7 (onset), 219.1 (peak) (DSC @ 5 °C/min) <sup>[1]</sup>		
ρ [g cm <sup>-3</sup> ]	1.786 (crystal) <sup>[1]</sup>		
Heat of formation	-395 kJ/mol (ΔH <sub>f</sub> <sup>o</sup> ) <sup>[1]</sup>		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
- Δ <sub>ex</sub> U <sup>o</sup> [kJ kg <sup>-1</sup> ]			

$T_{\text{ex}}$ [K]			
$p_{\text{CJ}}$ [kbar]		27.1 GPa (calcd., CHEETAH 7.0) <sup>[1]</sup>	
VoD [ $\text{m s}^{-1}$ ]		7,837 (@ 1.786 $\text{g cm}^{-3}$ , calcd., CHEETAH 7.0) <sup>[1]</sup>	
$V_0$ [ $\text{L kg}^{-1}$ ]			

	<b>BITN<sup>[1]</sup></b>
Chemical formula	$\text{C}_{10}\text{H}_8\text{N}_6\text{O}_{14}$
Molecular weight [g mol <sup>-1</sup> ]	436.22
Crystal system	Monoclinic
Space group	$P2_1$ (no. 4)
$a$ [\mathring{A}]	8.9329(5)
$b$ [\mathring{A}]	8.6103(4)
$c$ [\mathring{A}]	10.8182(4)
$\alpha$ [°]	90
$\beta$ [°]	102.847(5)
$\gamma$ [°]	90
$V$ [\mathring{A} <sup>3</sup> ]	811.25(7)
$Z$	2
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.7856
$T$ [K]	298

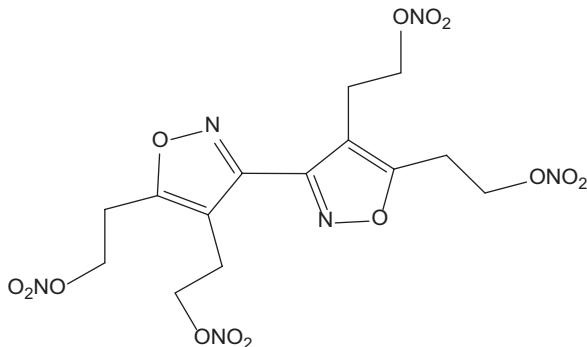
[1] L. A. Wingard, E. C. Johnson, p. E. Guzmán, J. J. Sabatini, G. W. Drake, E. F. C. Byrd, R. C. Sausa, *Eur. J. Org. Chem.*, **2017**, 1765–1768.

## [3,3'-Biisoxazole]-4,4',5,5'-tetrayltetrakis(ethane-2,1-diyl)tetranitrate

Name [German, acronym]: [3,3'-Biisoxazole]-4,4',5,5'-tetrayltetrakis(ethane-2,1-diyl)tetranitrate, [[3,3'-biisoxazol]-4,4',5,5'-tetrayltetrakis(ethan-2,1-diyl)tetranitrat, BITNE]

Main (potential) use: melt-cast

Structural formula:



	BITNE		
Formula	$\text{C}_{14}\text{H}_{16}\text{N}_6\text{O}_{14}$		
Molecular mass [g mol <sup>-1</sup> ]	492.31		
Appearance at RT	White solid <sup>[1]</sup>		
IS [J]	>36 (modified P.A. apparatus) <sup>[1]</sup>		
FS [N]	>350 (BAM) <sup>[1]</sup>		
ESD [J]	3.125 (firing test system model 931) <sup>[1]</sup>		
N [%]	17.07		
$\Omega(\text{CO}_2)$ [%]	-71.5		
$T_{\text{m.p.}}$ [°C]	69.5 <sup>[1]</sup>		
$T_{\text{dec.}}$ [°C]	183 <sup>[1]</sup>		
$\rho$ [g cm <sup>-3</sup> ]	1.568 (X-ray) <sup>[1]</sup>		
Heat of formation	-135.2 kJ/mol (calcd.) <sup>[1]</sup>		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^\circ$ [kJ kg <sup>-1</sup> ]			

$T_{\text{ex}}$ [K]			
$p_{\text{CJ}}$ [kbar]		19.6 GPa (calcd.) <sup>[1]</sup>	
VoD [m s <sup>-1</sup> ]		7,245 (@ 1.568 g cm <sup>-3</sup> , calcd.) <sup>[1]</sup>	
$V_0$ [L kg <sup>-1</sup> ]			
$I_{\text{sp}}$ [s]	205.7 (calcd.) <sup>[1]</sup>		
Compatibility	Hydrolytically stable <sup>[1]</sup>		

	<b>BITNE<sup>[1]</sup></b>
Chemical formula	C <sub>14</sub> H <sub>16</sub> N <sub>6</sub> O <sub>14</sub>
Molecular weight [g mol <sup>-1</sup> ]	492.31
Crystal system	Orthorhombic
Space group	Pbcn
$a$ [\AA]	27.3718(10)
$b$ [\AA]	10.9653(5)
$c$ [\AA]	6.9466(3)
$\alpha$ [°]	90
$\beta$ [°]	90
$\gamma$ [°]	90
$V$ [\AA <sup>3</sup> ]	2,084.95(15)
$Z$	4
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.568
$T$ [K]	298

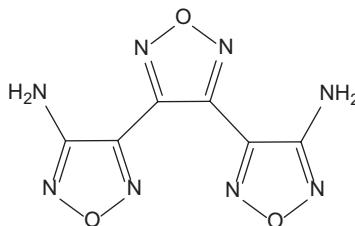
[1] L. A. Wingard, R. C. Sausa, P. E. Guzmán, R. Pesce-Rodriguez, J. J. Sabatini, G. W. Drake, *Propellants, Explosives, Pyrotechnics*, **2019**, *in press*.

**3,4-Bis(4'-aminofurazano-3') furoxan**

Name [German, acronym]: 4-[4-(4-Amino-1,2,5-oxadiazol-3-yl)-1,2,5-oxadiazol-3-yl]-1,2,5-oxadiazol-3-amine, [4-[4-(4-amino-1,2,5-oxadiazol-3-yl)-1,2,5-oxadiazol-3-yl]-1,2,5-oxadiazol-3-yl]-1,2,5-oxadiazol-3-amin]

Main (potential) use: high explosive

Structural formula:



	3,4-Bis(4-aminofurazano-3') furoxan		
Formula	C <sub>6</sub> H <sub>4</sub> N <sub>8</sub> O <sub>3</sub>		
Molecular mass [g mol <sup>-1</sup> ]	236.15		
Appearance at RT	White solid <sup>[1]</sup> , colorless prisms <sup>[1]</sup>		
IS [J]			
FS [N]			
ESD [J]			
N [%]	47.45		
Ω(CO <sub>2</sub> ) [%]	-74.5		
T <sub>m.p.</sub> [°C]	456–457 K <sup>[1]</sup>		
T <sub>dec.</sub> [°C]			
ρ [g cm <sup>-3</sup> ]	1.683 (X-ray @ 293 K) <sup>[1]</sup>		
Heat of formation			
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
-Δ <sub>ex</sub> U° [kJ kg <sup>-1</sup> ]			
T <sub>ex</sub> [K]			
p <sub>C-J</sub> [kbar]			
VoD [m s <sup>-1</sup> ]			
V <sub>0</sub> [L kg <sup>-1</sup> ]			

	<b>3,4-Bis(4-aminofurazano-3') furoxan<sup>[1]</sup></b>
Chemical formula	C <sub>6</sub> H <sub>4</sub> N <sub>8</sub> O <sub>3</sub>
Molecular weight [g mol <sup>-1</sup> ]	236.17
Crystal system	Monoclinic
Space group	C2/c
<i>a</i> [Å]	7.1681(9)
<i>b</i> [Å]	10.8147(13)
<i>c</i> [Å]	12.3448(18)
$\alpha$ [°]	90
$\beta$ [°]	103.155(1)
$\gamma$ [°]	90
<i>V</i> [Å <sup>3</sup> ]	931.9(2)
<i>Z</i>	4
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.683
<i>T</i> [K]	293

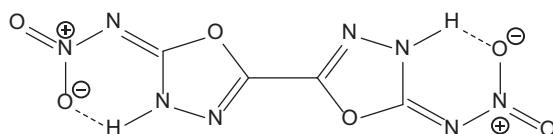
[1] S.-Y. Jia, B.-Z. Wang, X.-Z. Fan, P. Li, S. W. Ng, *Acta Cryst.*, **2012**, *68E*, 01573.

## [2,2'-Bi(1,3,4-oxadiazole)]-5,5'-dinitramide

Name [German, acronym]: [2,2'-Bi(1,3,4-oxadiazole)]-5,5'-dinitramide, [cM-101]

Main (potential) use: secondary explosive

Structural formula:



	ICM-101		
Formula	C <sub>4</sub> H <sub>2</sub> N <sub>8</sub> O <sub>6</sub>		
Molecular mass [g mol <sup>-1</sup> ]	258.01		
Appearance at RT	White solid <sup>[1]</sup>		
IS [J]	5 (BAM) <sup>[1]</sup>		
FS [N]	60 (BAM) <sup>[1]</sup>		
N [%]	43.41		
Ω(CO <sub>2</sub> ) [%]	6% (based on CO) <sup>[1]</sup>		
T <sub>m.p.</sub> [°C]			
T <sub>phase transition</sub> [°C]	No polymorphic transitions in temp. region 30–180 °C (X-ray powder diffraction) <sup>[1]</sup>		
T <sub>dec.</sub> [°C]	210.4 (onset, exo, dec.), 215.9 (peak max., exo, dec., DSC @ 10 °C/min) <sup>[1]</sup> , ~210 (dec. starts, TG @ 10 °C/min) <sup>[1]</sup> , 214.3 (thermal explosion, TG @ 10 °C/min) <sup>[1]</sup>		
ρ [g cm <sup>-3</sup> ]	2.038 (crystal @ 170 K) <sup>[1]</sup> , 1.990 (crystal @ 298 K) <sup>[1]</sup> , 1.9997 (gas pycnometry @ 298 K) <sup>[1]</sup>		
Heat of formation	166.8 kJ/mol (standard form. enthalpy, calcd., isodesmic, Gaussian) <sup>[1]</sup> , 159.52 kJ/mol (standard form. enthalpy, calcd. based on combustion enthalpy) <sup>[1]</sup>		
Heat of combustion	-2,035.50 kJ/mol (Δ <sub>c</sub> U, bomb calorimetry, @ C) <sup>[1]</sup> , -7,886 J/g (Δ <sub>c</sub> U, bomb calorimetry, @ C) <sup>[1]</sup>		
	Calcd. (EXPLO5 6.02)	Lit. values	Exptl.
- Δ <sub>ex</sub> U <sup>o</sup> [kJ kg <sup>-1</sup> ]			
T <sub>ex</sub> [K]			

$p_{\text{CJ}}$ [kbar]	41.9 GPa <sup>[1]</sup> 40.39 GPa (based on measured $\rho$ , and bomb calorimetry results) <sup>[1]</sup>		
VoD [ $\text{m s}^{-1}$ ]	9,481 <sup>[1]</sup> 9,475 (based on measured $\rho$ , and bomb calorimetry results) <sup>[1]</sup>		
$V_0$ [ $\text{L kg}^{-1}$ ]			
Solubility [g/mL]	Poorly soluble in $\text{H}_2\text{O}$ and most organic solvents <sup>[1]</sup> 0.26/100 g $\text{H}_2\text{O}$ <sup>[1]</sup> , 9/100 g DMSO <sup>[1]</sup> , 1/100 g DMF <sup>[1]</sup> , 0.11/100 g acetone <sup>[1]</sup> , 0.05/100 g $\text{CH}_2\text{Cl}_2$ <sup>[1]</sup> , 0.9/100 g $\text{CH}_3\text{OH}$ <sup>[1]</sup> , 0.01/100 g EtOAc <sup>[1]</sup> , 0.025/100 g EtOH <sup>[1]</sup> , 0.02/100 g $\text{CH}_3\text{CN}$ <sup>[1]</sup> , <0.01/100 g hexane <sup>[1]</sup> , <0.01/100 g $\text{Et}_2\text{O}$ <sup>[1]</sup>		
$\Delta_{\text{subl.}}U$ [kJ mol <sup>-1</sup> ]	90.80 <sup>[1]</sup>		

	ICM-101 <sup>[1]</sup>
Chemical formula	$\text{C}_4\text{H}_2\text{N}_8\text{O}_6$
Molecular weight [g mol <sup>-1</sup> ]	258.01
Crystal system	Orthorhombic
Space group	<i>Pbca</i>
$a$ [\mathring{A}]	6.4008(14)
$b$ [\mathring{A}]	8.3648(17)
$c$ [\mathring{A}]	16.094(3)
$\alpha$ [°]	90
$\beta$ [°]	90
$\gamma$ [°]	90
$V$ [\mathring{A} <sup>3</sup> ]	861.7(3)
$Z$	4
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.990 (@ 298 K) 2.037 (@ 170 K)
$T$ [K]	298

Crude product = irregular flake morphology (2–5  $\mu\text{m}$  particle size)<sup>[1]</sup>, crystals from DMSO = prism-like crystals (~400  $\mu\text{m}$  particle size in sites of severe agglomeration).<sup>[1]</sup>

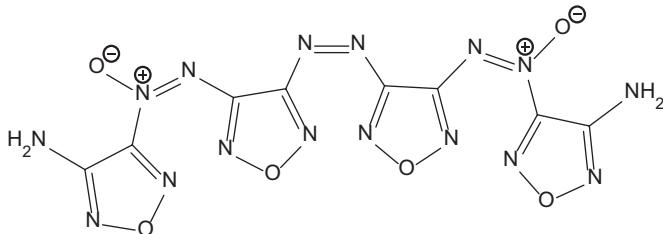
[1] W. Zhang, J. Zhang, M. Deng, X. Qi, F. Nie, Q. Zhang, *Nature Comm.*, **2017**, *8*, Article nr. 181 .

## Bis[4-aminofurazanyl-3-azoxy]azofurazan

Name [German, acronym]: Bis[4-aminofurazanyl-3-azoxy]azofurazan [ADAAF]

Main (potential) use: high explosive

Structural formula:



	<b>ADAAF</b>		
Formula	C <sub>8</sub> H <sub>4</sub> N <sub>16</sub> O <sub>6</sub>		
Molecular mass [g mol <sup>-1</sup> ]	420.23		
Appearance at RT	Yellow solid <sup>[1]</sup>		
IS [J]	$H_{50\%} = 36.2$ cm (2.5 kg mass, LANL type 12 test, Bruceton method) <sup>[1]</sup>		
FS [N]	26 kg (BAM, Bruceton, 50% load) <sup>[1]</sup>		
ESD [J]	0.0625 (ABL) <sup>[1]</sup>		
N [%]	53.33		
$\Omega(\text{CO}_2)$ [%]	-45.7		
T <sub>dec.</sub> [°C]	227 (exo, onset), 266 (exo, peak max.) (DSC @ 10 °C/min, hermetically sealed Al pans with pinhole lid, 1 mg sample) <sup>[1]</sup>		
$\rho$ [g cm <sup>-3</sup> ]	1.769 (calcd. @ 113 K) <sup>[1]</sup> , 1.728 (calcd. @ 293 K) <sup>[1]</sup> , 1.76 <sup>[1]</sup>		
Heat of formation	300 kcal/mol ( $\Delta_f H$ , combustion calorimetry) <sup>[1]</sup> , 237 kcal/mol ( $\Delta_f H$ , calcd.) <sup>[1]</sup>		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^0$ [kJ kg <sup>-1</sup> ]			
T <sub>ex</sub> [K]			

$p_{C_J}$ [kbar]		279 (@ 1.73 g cm <sup>-3</sup> , TMD, $\Delta H_f = 300$ kcal/mol, calcd., CHEETAH 4.0) <sup>[1]</sup> 244 (@ 1.63 g cm <sup>-3</sup> , 94% TMD, $\Delta H_f = 300$ kcal/mol, calcd., CHEETAH 4.0) <sup>[1]</sup> 298 (@ 1.76 g cm <sup>-3</sup> , calcd.) <sup>[1]</sup>	299 (@ 1.63 g cm <sup>-3</sup> , 94% TMD, rate stick of ADAAF pellets, 0.5 in diameter) <sup>[1]</sup>																					
VoD [m s <sup>-1</sup> ]		8,280 (@ 1.73 g cm <sup>-3</sup> , TMD, $\Delta H_f = 300$ kcal/mol, calcd., CHEETAH 4.0) <sup>[1]</sup> 7,890 (@ 1.63 g cm <sup>-3</sup> , 94% TMD, $\Delta H_f = 300$ kcal/mol, calcd., CHEETAH 4.0) <sup>[1]</sup> 8,090 (@ 1.76 g cm <sup>-3</sup> , calcd.) <sup>[1]</sup>	7,880 (@ 1.63 g cm <sup>-3</sup> , 94% TMD, rate stick of ADAAF pellets, 0.5 in diameter) <sup>[1]</sup>																					
$V_0$ [L kg <sup>-1</sup> ]																								
Burn rate [mm/s]	0.25 x 0.25 in cylindrical pellets, 93–94% TMD, pressurized combustion chamber filled with nitrogen between 0.3 and 7 MPa <sup>[1]</sup> :																							
	<table border="1"> <thead> <tr> <th>Pellet <math>\rho</math> (g cm<sup>-3</sup>)</th><th>Pressure (MPa)</th><th>Burning rate (mm/s)</th></tr> </thead> <tbody> <tr> <td>1.644</td><td>6.87</td><td>1.85</td></tr> <tr> <td>1.651</td><td>5.56</td><td>1.53</td></tr> <tr> <td>1.658</td><td>4.16</td><td>1.29</td></tr> <tr> <td>1.649</td><td>2.81</td><td>1.08</td></tr> <tr> <td>1.661</td><td>1.37</td><td>0.50</td></tr> <tr> <td>1.642</td><td>0.35</td><td>0.15</td></tr> </tbody> </table>			Pellet $\rho$ (g cm <sup>-3</sup> )	Pressure (MPa)	Burning rate (mm/s)	1.644	6.87	1.85	1.651	5.56	1.53	1.658	4.16	1.29	1.649	2.81	1.08	1.661	1.37	0.50	1.642	0.35	0.15
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1.658	4.16	1.29																						
1.649	2.81	1.08																						
1.661	1.37	0.50																						
1.642	0.35	0.15																						
Solubility [g/mL]	Solvent-free crystals obtained from hot acetonitrile <sup>[1]</sup>																							
Energy of dec. [J/g]	3,022 <sup>[1]</sup>																							

	<b>ADAAF<sup>[1]</sup></b>
Chemical formula	C <sub>8</sub> H <sub>4</sub> N <sub>16</sub> O <sub>6</sub>
Molecular weight [g mol <sup>-1</sup> ]	420.27
Crystal system	Monoclinic
Space group	P2 <sub>1</sub> /n
a [Å]	11.309(14)
b [Å]	11.3388(5)
c [Å]	12.7226(5)
α [°]	90
β [°]	104.11(6)
γ [°]	90
V [Å <sup>3</sup> ]	1,577.60(11)
Z	4
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.769 (calcd. @ 113 K) 1.728 (calcd. @ 293 K)
T [K]	113

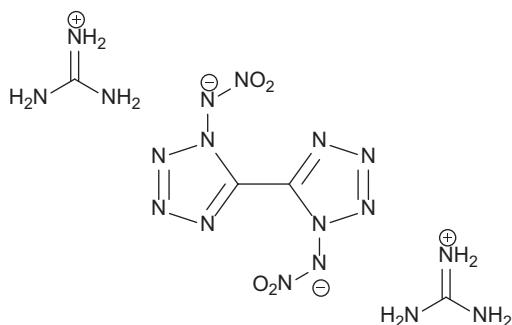
[1] J. M. Veauthier, D. E. Chavez, B. C. Tappan, D. A. Parrish, *J. Energet. Mater.*, **2010**, *28*, 229–249.

**Bis(aminoguanidinium) 1,1'-dinitramino-5,5'-bitetrazolate**

Name [acronym]: Bis(aminoguanidinium) 1,1'-dinitramino-5,5'-bitetrazolate  
[(AG)2DNABT]

Main (potential) use: Secondary (primary) explosive

Structural formula:



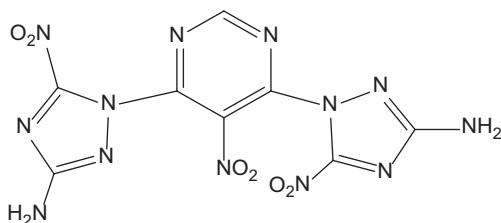
	(AG)2DNABT	
Formula	C <sub>4</sub> H <sub>14</sub> N <sub>20</sub> O <sub>4</sub>	
Molecular mass [g mol <sup>-1</sup> ]	406.35	
Appearance at RT		
IS [J]	3.9	
FS [N]	80	
N [%]	68.9	
Ω(CO <sub>2</sub> ) [%]	-43.3	
T <sub>m,p.</sub> [°C]	159.2	
T <sub>dec.</sub> [°C]	180.0 (DSC @ 5 °C/min)	
ρ [g cm <sup>-3</sup> ]	1.69 (@ 298 K)	
Heat of formation	880.0 kJ/mol (ΔH <sup>o</sup> <sub>f</sub> )	
	Calcd.	Exptl.
-Δ <sub>ex</sub> U <sup>o</sup> [kJ kg <sup>-1</sup> ]	4,542	
T <sub>ex</sub> [K]		
p <sub>CJ</sub> [kbar]	281	
VoD [m s <sup>-1</sup> ]	8,116 (@ TMD)	
V <sub>0</sub> [L kg <sup>-1</sup> ]		

**4,6-Bis-(3-amino-5-nitro-1*H*-1,2,4-triazole-1-yl)-5-nitropyrimidine**

Name [German, acronym]: 4,6-Bis(5-amino-3-nitro-1,2,4-triazolyl)-5-nitropyrimidine, 4,6-bis(5-amino-3-nitro-1*H*-1,2,4-triazol-1-yl)-5-nitropyrimidine, 5-nitro-4,6-bis(5-amino-3-nitro-1*H*-1,2,4-triazol-1-yl)pyrimidine [DANTNP]

Main (potential) use: Possible future as component of propellant and explosive formulations where the combination of insensitivity and thermal stability is important<sup>[1]</sup>, developed as insensitive energetic compound<sup>[5]</sup>

Structural formula:



	DANTNP
Formula	C <sub>8</sub> H <sub>5</sub> N <sub>13</sub> O <sub>6</sub>
Molecular mass [g mol <sup>-1</sup> ]	379.21
Appearance at RT	
IS [J]	>170 cm (2 kg mass, Bruceton method) <sup>[1]</sup> , >320 cm (type 12) <sup>[3]</sup> , H <sub>50%</sub> = >170 cm <sup>[7]</sup>
ESD [J]	>1.0 (3 mil foil) <sup>[3]</sup>
N [%]	48.02
Ω(CO <sub>2</sub> ) [%]	-52.7
T <sub>m.p.</sub> [°C]	>330 <sup>[1,7]</sup> , 330 <sup>[2]</sup> , does not melt but begins dec. @ 300 °C (DTA) <sup>[3]</sup> , 350 (dec.) <sup>[5]</sup>
T <sub>dec.</sub> [°C]	317 (exo, DTA) <sup>[1]</sup> , 290 (onset of mass loss, DTA, sharp weight loss (73%) up to 320 °C, slow weight loss after 320 °C, total weight loss = 89% up to 600 °C) <sup>[1]</sup> , 341 (exo, peak max., DSC @ 10 °C/min) <sup>[1]</sup> , 344 (exo, peak max., DSC @ 15 °C/min) <sup>[1]</sup> , 347 (exo, peak max., DSC @ 20 °C/min) <sup>[1]</sup> , 349 (exo, peak max., DSC @ 25 °C/min) <sup>[1]</sup> , 300 (dec. begins, DTA) <sup>[3]</sup>
ρ [g cm <sup>-3</sup> ]	1.84 <sup>[1,7]</sup> , 1.865 <sup>[2]</sup> , 1.84 (gas pycnometry) <sup>[3]</sup> , 1.84 (crystal) <sup>[6]</sup> , 1.818 (calcd., EDPHT 2.0) <sup>[6]</sup> , 1.882 (calcd., Ammon) <sup>[6]</sup>
Heat of formation	103 ± 5 kcal/mol <sup>[3]</sup> , 430 ± 20 kJ/mol ( $\Delta_f H^\circ (s)$ ) <sup>[4]</sup>

	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^{\circ} [\text{kJ kg}^{-1}]$			
$T_{\text{ex}} [\text{K}]$			
$p_{\text{CJ}} [\text{kbar}]$		297 (@ 1.84 g cm <sup>-3</sup> , $\Delta H_f = 103 \text{ kcal/mol}$ , calcd., BKW) <sup>[3]</sup>	327 (@ 1.87 g cm <sup>-3</sup> ) <sup>[5]</sup>
VoD [m s <sup>-1</sup> ]		8,120 (@ 1.84 g cm <sup>-3</sup> , $\Delta H_f = 103 \text{ kcal/mol}$ , calcd., BKW) <sup>[3]</sup>	8,200 (@ 1.87 g cm <sup>-3</sup> ) <sup>[5]</sup>
$V_0 [\text{L kg}^{-1}]$			
$\Delta E_{\text{dec}} [\text{J/g}]$	1,356 (DSC @ 10 °C/min) <sup>[1]</sup>		
Performance	10% greater than TATB <sup>[2]</sup>		

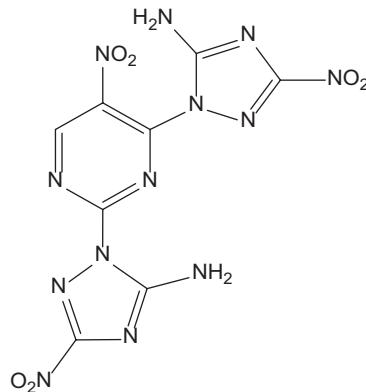
- [1] A. K. Sikder, M. Geetha, D. B. Sarwade, J. P. Agrawal, *J. Hazard. Mater.*, **2001**, *A82*, 1–12.
- [2] P. F. Pagoria, G. S. Lee, A. R. Mitchell, R. D. Schmidt, *Thermochim. Acta*, **2002**, *384*, 187–204.
- [3] K.-Y. Lee, C. B. Storm, M. A. Hiskey, M. D. Coburn, *J. Energet. Mater.*, **1991**, *9*, 415–428.
- [4] P. J. Lindstrom, W. G. Mallard, *NIST Chemistry WebBook*, NIST Standard Reference Database, National Institute of Standards and Technology, Gaithersburg, USA, webbook.nist.gov.
- [5] G. Subramanian, G. Eck, J. H. Boyer, E. D. Stevens, M. L. Trudell, *J. Org. Chem.*, **1996**, *61*, 5801–5803.
- [6] M. H. Keshavarz, H. Motamedshariati, R. Moghayadnia, M. Ghanbarzadeh, J. Azarniamehraban, *Propellants, Explosives, Pyrotechnics*, **2013**, *38*, 95–102.
- [7] T. M. Klapötke, J. M. Short, *Energetics in the Rest of the World*, ch. 4 in *Topics in Energetics—Research and Development*, CALCE Press, University of Maryland, Maryland, USA, **2013**.

## 2,4-Bis(5-amino-3-nitro-1,2,4-triazolyl)pyrimidine

Name [German, acronym]: 2,4-Bis(5-amino-3-nitro-1,2,4-triazolyl)pyrimidine  
 [2,4-bis(5-amino-3-nitro-1,2,4-triazolyl)pyrimidin, IHNX]

Main (potential) use: explosive

Structural formula:



	IHNX		
Formula	$C_8H_5N_{13}O_6$		
Molecular mass [g mol <sup>-1</sup> ]	379.21		
Appearance at RT			
IS [J]			
FS [N]			
ESD [J]			
N [%]	48.02		
$\Omega(CO_2)$ [%]	-52.7		
$T_{m.p.}$ [°C]			
$T_{dec.}$ [°C]			
$\rho$ [g cm <sup>-3</sup> ]			
Heat of formation			
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{ex}U^\circ$ [kJ kg <sup>-1</sup> ]			

$T_{\text{ex}}$ [K]			
$p_{\text{CJ}}$ [kbar]			
VoD [ $\text{m s}^{-1}$ ]			
$V_0$ [ $\text{L kg}^{-1}$ ]			

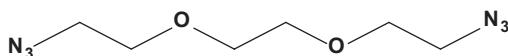
- [1] R. D. Schmidt, G. S. Lee, P. F. Pagoria, A. R. Mitchell, R. Gilardi, *Synthesis and Properties of a New Explosive, 4-Amino-3,5-dinitro-1H-pyrazole (LLM-116)*, UCRL-ID-148510, LLNL, USA, May 22nd 2001.

## 1,2-Bis(2-azidoethoxy)ethane

Name [German, acronym]: Bis-azido-triethyleneglycol [TEGDA, TEG, BATEG]

Main (potential) use: Energetic plasticizer<sup>[2]</sup>

Structural formula:



	TEGDA		
Formula	C <sub>6</sub> H <sub>12</sub> N <sub>6</sub> O <sub>2</sub>		
Molecular mass [g mol <sup>-1</sup> ]	200.21		
Appearance at RT	Pale yellow-brown liquid		
N [%]	41.98		
Ω(CO <sub>2</sub> ) [%]	-127.9		
T <sub>glass transition</sub> [°C]	-111 (DSC @ 10 °C, hermetically closed Al crucible) <sup>[2]</sup>		
T <sub>dec.</sub> [°C]			
ρ [g cm <sup>-3</sup> ]	1.15 <sup>[2]</sup>		
Heat of formation	160 kJ/mol (Δ <sub>f</sub> H <sup>o</sup> ) <sup>[1]</sup>		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
-Δ <sub>ex</sub> U <sup>o</sup> [kJ kg <sup>-1</sup> ]			
T <sub>ex</sub> [K]			
p <sub>C,J</sub> [kbar]			
VoD [m s <sup>-1</sup> ]			
V <sub>0</sub> [L kg <sup>-1</sup> ]			

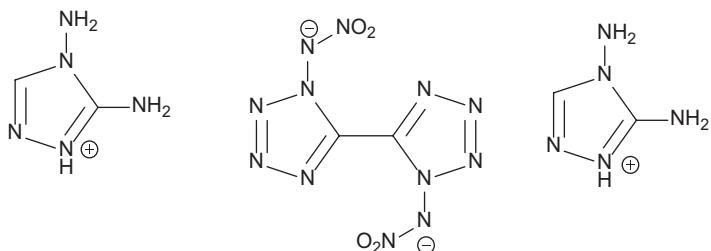
- [1] M. F. Lemos, M. A. Bohn, L. C. Mendes, *Compatibility Between Azido Groups Containing Molecules and HTPB*, in *Proc. 48th Int. Annual Conf. of ICT*, 27th–30th June 2017, Karlsruhe, Germany, pp. 102–1–102–11.
- [2] M. F. Lemos, M. A. Bohn, *The Effect of Plasticizers on the Glass-to-Rubber Behavior of Desmophen® 2200 Based Elastomers Used for Composite Propellants*, in *46th Int. Annual Conf. of ICT*, 23rd–26th June 2015, Karlsruhe, Germany, pp. 22-1–22-26.

**Bis(3,4-diamino-1,2,4-triazolium)  
1,1'-dinitramino-5,5'-bitetrazolate**

Name [acronym]: Bis(3,4-diamino-1,2,4-triazolium) 1,1'-dinitramino-5, 5'-bitetrazolate [(DATr)<sub>2</sub>DNABT]

Main (potential) use: Secondary (primary) explosive

Structural formula:



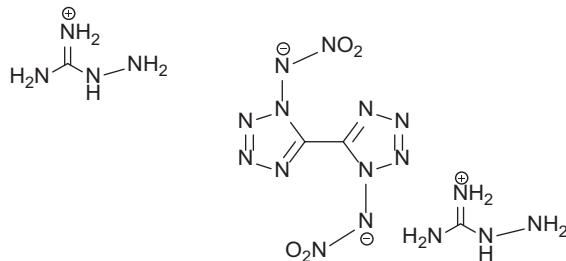
	(DATr) <sub>2</sub> DNABT	
Formula	C <sub>6</sub> H <sub>12</sub> N <sub>22</sub> O <sub>4</sub>	
Molecular mass [g mol <sup>-1</sup> ]	456.38	
Appearance at RT		
IS [J]	4.9	
FS [N]	96	
N [%]	67.5	
Ω(CO <sub>2</sub> ) [%]	-49.0	
T <sub>m.p.</sub> [°C]		
T <sub>dec.</sub> [°C]	183.1 (DSC @ 5 °C/min)	
ρ [g cm <sup>-3</sup> ]	1.75 (@ 298 K)	
Heat of formation	1,324.3 kJ/mol (ΔH <sup>o</sup> <sub>f</sub> )	
	Calcd.	Exptl.
-Δ <sub>ex</sub> U <sup>o</sup> [kJ kg <sup>-1</sup> ]	5,017	
T <sub>ex</sub> [K]		
p <sub>CJ</sub> [kbar]	292	
VoD [m s <sup>-1</sup> ]	8,182 (@ TMD)	
V <sub>0</sub> [L kg <sup>-1</sup> ]		

**Bis(diaminouronium) 1,1'-dinitramino-5,5'-bitetrazolate**

Name [acronym]: Bis(diaminouronium) 1,1'-dinitramino-5,5'-bitetrazolate  
[(CHZ)<sub>2</sub>DNABT]

Main (potential) use: Secondary (primary) explosive

Structural formula:



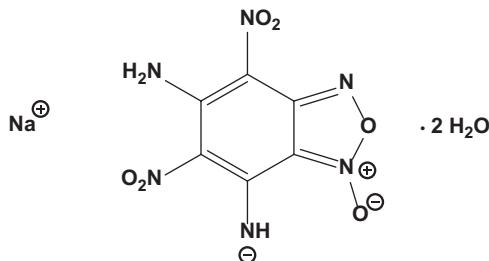
	<b>(CHZ)<sub>2</sub>DNABT</b>	
Formula	C <sub>4</sub> H <sub>14</sub> N <sub>20</sub> O <sub>6</sub>	
Molecular mass [g mol <sup>-1</sup> ]	438.35	
Appearance at RT		
IS [J]	2.5	
FS [N]	40	
N [%]	63.8	
Ω(CO <sub>2</sub> ) [%]	-32.8	
T <sub>m.p.</sub> [°C]		
T <sub>dec.</sub> [°C]	184.6	
ρ [g cm <sup>-3</sup> ]	1.77 (@ 298 K)	
Heat of formation	773.6 kJ/mol (ΔH <sup>o</sup> <sub>f</sub> )	
	Calcd.	Exptl.
-Δ <sub>ex</sub> U <sup>o</sup> [kJ kg <sup>-1</sup> ]	5,070	
T <sub>ex</sub> [K]		
p <sub>CJ</sub> [kbar]	315	
VoD [m s <sup>-1</sup> ]	8,477 (@ TMD)	
V <sub>0</sub> [L kg <sup>-1</sup> ]		

## 5,7-Diamino-4,6-dinitrobenzofuroxan dihydrate, sodium salt

Name [German, acronym]: 5,7-Diamino-4,6-dinitrobenzofuroxan dihydrate, sodium salt [Natrium 5,7-Diamino-4,6-dinitrobenzofuroxan dihydrat, Na[CL-14 · 2H<sub>2</sub>O]]

Main (potential) use: Proposed as potential energetic catalyst in AN-based propellants<sup>[1]</sup>

Structural formula:



	Na[CL-14 · 2H <sub>2</sub> O]										
Formula	C <sub>6</sub> H <sub>7</sub> N <sub>6</sub> NaO <sub>8</sub>										
Molecular mass [g mol <sup>-1</sup> ]	314.15										
Appearance at RT	Yellow crystals <sup>[1]</sup>										
IS [J]	27 (BAM) <sup>[1]</sup>										
FS [N]	360 (BAM) <sup>[1]</sup>										
N [%]	26.75										
Ω(CO <sub>2</sub> ) [%]											
T <sub>m.p.</sub> [°C]	103.5 (endo peak max., DSC @ 5 °C/min) <sup>[1]</sup>										
T <sub>dec.</sub> [°C]	306.3 (exo peak max., 268.6 °C onset, DSC @ 5 °C/min) <sup>[1]</sup>  DSC data from <sup>[1]</sup> :  <table border="1"> <thead> <tr> <th>β (°C/min)</th> <th>T<sub>p</sub> (K)</th> </tr> </thead> <tbody> <tr> <td>2.5</td> <td>570.24</td> </tr> <tr> <td>5</td> <td>579.41</td> </tr> <tr> <td>10</td> <td>582.75</td> </tr> <tr> <td>20</td> <td>590.79</td> </tr> </tbody> </table>	β (°C/min)	T <sub>p</sub> (K)	2.5	570.24	5	579.41	10	582.75	20	590.79
β (°C/min)	T <sub>p</sub> (K)										
2.5	570.24										
5	579.41										
10	582.75										
20	590.79										
ρ [g cm <sup>-3</sup> ]	1.942 (X-ray @ 293 K) <sup>[1]</sup>										
Heat of formation											

	Calcd. (EXPL05 6.04)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^{\circ}$ [kJ kg <sup>-1</sup> ]			
$T_{\text{ex}}$ [K]			
$p_{\text{CJ}}$ [kbar]			
VoD [m s <sup>-1</sup> ]			
$V_0$ [L kg <sup>-1</sup> ]			
Thermal stability	268.6–338.5 (52.0% mass loss, TG) <sup>[1]</sup> , 338.5–400 °C (slow mass loss of 3.95%, TG) <sup>[1]</sup>		
Solubility [g/mL]	Soluble in MeOH <sup>[1]</sup>		
$\Delta H_{\text{dec}}$ [J/g]	1,848 (DSC @ 5 °C/min) <sup>[1]</sup>		

	<b>Na[CL-14·2H<sub>2</sub>O]<sup>[1]</sup></b>
Chemical formula	C <sub>6</sub> H <sub>7</sub> NaN <sub>6</sub> O <sub>8</sub>
Molecular weight [g mol <sup>-1</sup> ]	314.17
Crystal system	Monoclinic
Space group	P2 <sub>1</sub> /c (no. 14)
<i>a</i> [Å]	13.087(3)
<i>b</i> [Å]	13.021(3)
<i>c</i> [Å]	6.3070(13)
$\alpha$ [°]	90
$\beta$ [°]	90.56(3)
$\gamma$ [°]	90
<i>V</i> [Å <sup>3</sup> ]	1,074.7(4)
<i>Z</i>	4
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.942
<i>T</i> [K]	293

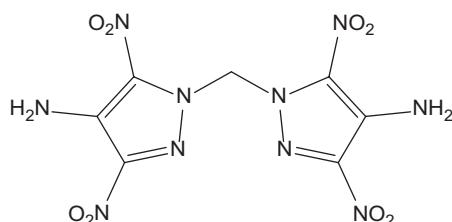
[1] J. Cheng, Y. Dong, H. Ma, L. Li, Z. Liu, F. Zhao, S. Xu, *RSC Adv.*, **2015**, *5*, 64358–64367.

## Bis(3,5-dinitro-4-aminopyrazolyl)methane

Name [German, acronym]: Bis(3,5-dinitro-4-aminopyrazolyl)methane [BDNAPM]

Main (potential) use: Thermally stable high explosive

Structural formula:



	<b>BDNAPM</b>		
Formula	C <sub>7</sub> H <sub>6</sub> N <sub>10</sub> O <sub>8</sub>		
Molecular mass [g mol <sup>-1</sup> ]	358.2		
IS [J]	11 <sup>[1]</sup>		
FS [N]	>360 <sup>[1]</sup>		
ESD [J]	>1 <sup>[1]</sup>		
N [%]	39.10		
Ω(CO <sub>2</sub> ) [%]	-40.20		
T <sub>dec.</sub> [°C]	310 (DSC @ 5 °C/min) <sup>[1]</sup>		
ρ [g cm <sup>-3</sup> ]	1.802 (@ 298 K) <sup>[1]</sup> , 1.836 (X-ray @ 173 K) <sup>[1]</sup>		
Heat of formation	205.1 kJ/mol (ΔH <sup>o</sup> <sub>f</sub> ) <sup>[1]</sup> , 655.8 kJ kg <sup>-1</sup> (ΔH <sup>o</sup> <sub>f</sub> ) <sup>[1]</sup>		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
-Δ <sub>ex</sub> U <sup>o</sup> [kJ kg <sup>-1</sup> ]	4721		
T <sub>ex</sub> [K]	3,448		
p <sub>CJ</sub> [kbar]	277		
VoD [m s <sup>-1</sup> ]	8,132 (@ 1.802 g cm <sup>-3</sup> )	8,171 (@ TMD, calcd., CHEETAH v8.0) <sup>[2]</sup>	8,630 ± 210 (est., LASEM method) <sup>[2]</sup>
V <sub>0</sub> [L kg <sup>-1</sup> ]	709		

	<b>BDNAPM<sup>[1]</sup></b>
Chemical formula	C <sub>7</sub> H <sub>6</sub> N <sub>10</sub> O <sub>8</sub>
Molecular weight [g mol <sup>-1</sup> ]	358.22
Crystal system	Orthorhombic
Space group	<i>Pbca</i> (no. 61)
<i>a</i> [Å]	12.2107(8)
<i>b</i> [Å]	9.6010(7)
<i>c</i> [Å]	22.1100(12)
$\alpha$ [°]	90
$\beta$ [°]	90
$\gamma$ [°]	90
<i>V</i> [Å <sup>3</sup> ]	1,592.1(3)
<i>Z</i>	8
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.836
<i>T</i> [K]	173

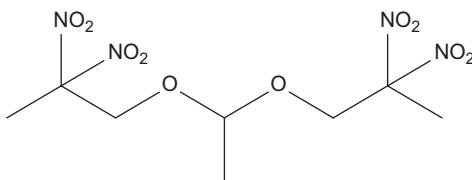
- [1] D. Fischer, J. L. Gottfried, T. M. Klapötke, K. Karaghiosoff, J. Stierstorfer, T. G. Witkowski, *Angew Chem. Int. Ed.*, **2016**, *55*, 16132–16135.  
[2] J. L. Gottfried, T. M. Klapötke, T. G. Witkowski, *Propellants, Explosives, Pyrotechnics*, **2017**, *42*, 353–359.

## Bis(2,2-dinitropropyl)acetal

Name [German, acronym]: Bis(2,2-dinitropropyl)acetal, 1,1-bis(2,2-dinitropropoxy)ethane, tetranitro-5-methyl-4,6-dioxanonane, 1-[1-(2,2-dinitropropoxy)ethoxy]-2,2-dinitropropane [BDNPA]

Main (potential) use: Plasticizer for nitrocellulose and polyurethanes<sup>[1]</sup>

Structural formula:



	<b>BDNPA</b>
Formula	$\text{C}_8\text{H}_{14}\text{N}_4\text{O}_{10}$
Molecular mass [g mol <sup>-1</sup> ]	326.22
Appearance at RT	
IS [J]	96 cm <sup>[5]</sup> , 170 (Julius-Peters apparatus) <sup>[6]</sup>
FS [N]	>36 kg (Julius-Peters apparatus) <sup>[6]</sup>
N [%]	17.18
$\Omega(\text{CO}_2)$ [%]	-63.8
$T_{\text{m.p.}}$ [°C]	28–29 <sup>[1]</sup> , 33–35 <sup>[6]</sup>
$T_{\text{b.p.}}$ [°C]	150 (@ 0.01 mm Hg) <sup>[6]</sup>
$T_{\text{dec.}}$ [°C]	248 (exo peak max, DTA @ 10 °C/min, 10 mg sample, in air) <sup>[6]</sup>
$\rho$ [g cm <sup>-3</sup> ]	$1.450 \pm 0.06$ (@ 293.15 K) <sup>[2]</sup> , 1.342 <sup>[4]</sup> , 1.36 (@ 27 °C) <sup>[6]</sup>
Heat of formation	$-641.83 \text{ kJ/mol}$ ( $\Delta H^\circ_f$ ) <sup>[3]</sup> , $-1,967.46 \text{ kJ kg}^{-1}$ ( $\Delta H^\circ_f$ ) <sup>[3]</sup> , $-1,966.5 \text{ kJ/kg}$ <sup>[4]</sup> , $-484 \text{ cal/g}$ <sup>[6]</sup>
Calcd. (EXPLO5 6.04)	Exptl.
$-\Delta_{\text{ex}}U^\circ$ [kJ kg <sup>-1</sup> ]	4,170
$T_{\text{ex}}$ [K]	2,902

$p_{C_J}$ [GPa]	14.6	
VoD [ $\text{m s}^{-1}$ ]	6,521 (@ 1.35 g $\text{cm}^{-3}$ , $\Delta_f H = -652 \text{ kJ mol}^{-1}$ )	
$V_0$ [ $\text{L kg}^{-1}$ ]	824	

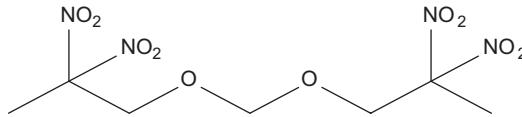
Vapor pressure [atm. @ °C]	$1.4532 + 0.40/-0.27 \text{ mPa}^{[7]}$
$\Delta_{\text{vap}}H$ [kJ mol $^{-1}$ ]	$93.01 \pm 0.38^{[7]}$

- [1] M. H. Gold, H. J. Marcus, *Nitro Acetals*, US Patent 3291833A, **1963**.
- [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. 30.
- [4] <https://engineering.purdue.edu/~propulsi/propulsion/comb/propellants.html>
- [5] *Chemical Rocket Propulsion: A Comprehensive Survey of Energetic Materials*, L. DeLuca, T. Shimada, V. P. Sinditskii, M. Calabro (eds.), Springer, **2017**.
- [6] G. M. Gore, R. G. Bhatewara, K. R. Tipare, N. M. Walunj, V. K. Bhat, *BDNPA/F as Energetic Plasticizer in Propellant Formulations*, ICT **1998**, Karlsruhe, Germany, pp. 136-1–136-12.
- [7] R. B. Rauch, R. Behrens, *Propellants, Explosives, Pyrotechnics*, **2007**, 32, 97–116.

## Bis(2,2-dinitropropyl)formal

Name [German, acronym]: Bis(2,2-dinitropropyl)formal [BDNPF, DNPFO]  
 Main (potential) use: Plasticizer for polyurethane binders for solid rocket fuels<sup>[1]</sup>

Structural formula:



	<b>BDNPF</b>
Formula	C <sub>7</sub> H <sub>12</sub> N <sub>4</sub> O <sub>10</sub>
Molecular mass [g mol <sup>-1</sup> ]	312.19
Appearance at RT	
IS [J]	170 cm (Julius-Peters apparatus) <sup>[8]</sup> , 177 cm (LLL, cf. NG = 19.8 cm, open plate) <sup>[10]</sup> , H <sub>50%</sub> = 180 cm (2.5 kg mass, type 12 tool, ERL method) <sup>[11]</sup>
FS [N]	>36 kg (Julius-Peters apparatus) <sup>[8]</sup>
N [%]	17.95
Ω(CO <sub>2</sub> ) [%]	-51.3
T <sub>m.p.</sub> [°C]	32.5–33.5 <sup>[1]</sup> , 31 <sup>[3,8]</sup> , 33 <sup>[10]</sup>
T <sub>b.p.</sub> [°C]	149 (@ 0.01 mm Hg) <sup>[8]</sup>
T <sub>dec.</sub> [°C]	248 (exo peak max, DTA @ 10 °C/min, 10 mg sample in air) <sup>[8]</sup> , 215 (exo, DTA @ 10 °C/min, open Al pan) <sup>[10]</sup>
ρ [g cm <sup>-3</sup> ]	1.500 ± 0.06 (@ 293.15 K) <sup>[2]</sup> , 1.414 <sup>[4]</sup> , 1.41 (@ 27 °C) <sup>[8]</sup> , 1.39 (@ TMD (liq.)) <sup>[9]</sup> , 1.56 <sup>[10]</sup>
Heat of formation	-597.06 kJ/mol (ΔH <sup>o</sup> <sub>f</sub> ) <sup>[3]</sup> , -1,912.46 kJ kg <sup>-1</sup> (ΔH <sup>o</sup> <sub>f</sub> ) <sup>[3]</sup> , -1,912.1 kJ kg <sup>-1</sup> <sup>[4]</sup> , 457 cal/g (H <sub>f</sub> ) <sup>[8]</sup> , -597.1 kJ/mol <sup>[9]</sup> , -143 kcal/mol (ΔH <sub>f</sub> ) <sup>[10]</sup> , -475 kJ/mol (ΔH <sub>f</sub> (s), Byrd and Rice method) <sup>[5]</sup> , -461.0 kJ/mol (ΔH <sub>f</sub> (g), isodesmic rxn. method) <sup>[5]</sup>
Calcd. (EXPLO 6.04)	Lit. values
- Δ <sub>ex</sub> U <sup>o</sup> [kJ kg <sup>-1</sup> ]	4,428
T <sub>ex</sub> [K]	3,141

$p_{C_J}$ [GPa]	17.2	23.9 <sup>[5]</sup> 246 kbar (calcd., TIGER) <sup>[10]</sup> 191 kbar (calcd., K-J) <sup>[10]</sup>	
$\Delta_f H$ [ $\text{m s}^{-1}$ ]	6,786 (@ 1.4 g cm <sup>-3</sup> , $\Delta_f H = -597 \text{ kJ mol}^{-1}$ )	7,530 (@ 1.59 g cm <sup>-3</sup> ) <sup>[5]</sup>	
$V_0$ [L kg <sup>-1</sup> ]	812	196.2 cm <sup>3</sup> /mol <sup>[5]</sup>	

Vapor pressure [atm. @ °C]	2.20 + 1.87/ $-1.07 \text{ mPa}^{[7]}$
$\Delta_{\text{vap}}H$ [kJ mol <sup>-1</sup> ]	84.77 ± 0.88 <sup>[7]</sup>

	<b>BDNPF<sup>[6]</sup></b>
Chemical formula	C <sub>7</sub> H <sub>12</sub> N <sub>4</sub> O <sub>10</sub>
Molecular weight [g mol <sup>-1</sup> ]	312.21
Crystal system	Monoclinic
Space group	C2/c
$a$ [Å]	23.330(3)
$b$ [Å]	6.207(3)
$c$ [Å]	10.009(6)
$\alpha$ [°]	90
$\beta$ [°]	109.60(3)
$\gamma$ [°]	90
$V$ [Å <sup>3</sup> ]	1,365.6(11)
$Z$	4
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.519
$T$ [K]	291

- [1] M. H. Gold, H. J. Marcus, *Nitro Acetals*, US Patent 3291833A, **1963**.
- [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. 31.
- [4] <https://engineering.purdue.edu/~propuls/propulsion/comb/propellants.html>
- [5] R.-Z. Zhang, X.-H. Li, *Chinese J. Struct. Chem.*, **2014**, 33, 71–78.
- [6] F. Liu, H. Dai, Z. Huang, Y. Liu, X. Kou, *Acta Cryst.*, **2009**, E65, 0903.
- [7] R. B. Rauch, R. Behrens, *Propellants, Explosives, Pyrotechnics*, **2007**, 32, 97–116.

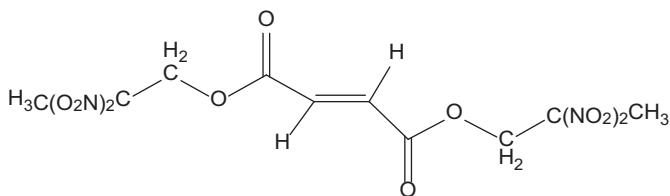
- [8] G. M. Gore, R. G. Bhatewara, K. R. Tipare, N. M. Walunj, V. K. Bhat, *BDNPA/F as Energetic Plasticizer in Propellant Formulations*, ICT 1998, Karlsruhe, Germany, pp. 136-1–136-12.
- [9] P. C. Souers, J. W. Kury, *Propellants, Explosives, Pyrotechnics*, 1993, 18, 175–183.
- [10] M. E. Hill, J. M. Guimont, *Desensitization of Explosive Materials*, ADA082893, Office of Naval Research, Maryland, USA, April 9th 1980.
- [11] J. Wenograd, *The Thermal Sensitivity of Explosives and Propellants*, US Naval Ordnance Laboratory, White Oak, Maryland, USA, NOLTR 61-97, 1st September 1961.

## Bis(2,2-dinitropropyl)fumarate

Name [German, acronym]: Bis(dinitropropyl) fumarate [DNPF, FUM]

Main (potential) use: Patented as an energetic binder component of a melt cast explosive<sup>[2]</sup>, ingredient of HE shell and bomb filler and as explosive desensitizer<sup>[3]</sup>

Structural formula:



	DNPF		
Formula	$\text{C}_{10}\text{H}_{12}\text{N}_4\text{O}_{12}$		
Molecular mass [g mol <sup>-1</sup> ]	380.22		
Appearance at RT	White crystals <sup>[3]</sup>		
IS [J]	100+ cm (2 kg mass, 20 mg sample, B.M.) <sup>[1]</sup> , 18 in (2 kg mass, 18 mg sample, P.A.) <sup>[1]</sup> , $H_{50\%} = 276.1$ cm (2.5 kg mass, 35 mg sample, 25 trials, type 12 tool, Gen Rad noisemeter, 180A garnet paper, ERL Bruceton apparatus) <sup>[2]</sup> , >600 mm (three consecutive positive trials, 5 kg mass) <sup>[2]</sup>		
FS [N]	Unaffected by steel shoe (friction pendulum test) <sup>[1]</sup> , unaffected by fiber shoe (friction pendulum test) <sup>[1]</sup> , >980 psig (sliding friction, 8 ft./s., 20 Til, threshold friction level) <sup>[2]</sup>		
ESD [J]	>12.5 (500 V, 20 Til) <sup>[2]</sup>		
N [%]	14.74		
$\Omega(\text{CO}_2)$ [%]	-59		
$T_{\text{m.p.}}$ [°C]	89 (form I) <sup>[1]</sup> , 86 (form II) <sup>[1]</sup> , 84 <sup>[2]</sup>		
$T_{\text{dec.}}$ [°C]			
$\rho$ [g cm <sup>-3</sup> ]	1.60 (crystal) <sup>[1]</sup> , 1.50 (loading density) <sup>[1]</sup> , 1.382 (liquid density @ 98.9 °C) <sup>[1]</sup> , 1.375 (liquid density @ 106.5 °C) <sup>[1]</sup>		
Heat of formation			
Heat of combustion	3,070 cal/g (calcd.) <sup>[1]</sup>		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.

$-\Delta_{\text{ex}}U^0$ [kJ kg <sup>-1</sup> ]		767 cal/g (calcd.) <sup>[1]</sup>	
$T_{\text{ex}}$ [K]			
$p_{\text{CJ}}$ [kbar]			
VoD [m s <sup>-1</sup> ]			6,050 (@ 1.49 g cm <sup>-3</sup> ) <sup>[1]</sup>
$V_0$ [L kg <sup>-1</sup> ]			
5 s explosion $T$ [°C] Explosion $T$ [°C]		250 (smokes) <sup>[1]</sup>	
Vacuum stability test [cm <sup>3</sup> /h]		0.66 cc/40 h @ 100 °C <sup>[1]</sup> , 0.91 cc/40 h @ 135 °C <sup>[1]</sup>	
Viscosity [Poises]		0.586 @ 98.9 °C <sup>[1]</sup> , 0.435 @ 106.5 °C <sup>[1]</sup>	
Solubility [g/mL]		Recryst. from MeOH <sup>[1]</sup>	

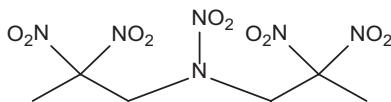
- [1] *AMC Pamphlet Engineering Design Handbook: Explosive Series Properties of Explosives of Military Interest*, Headquarters, U.S. Army Materiel Command, January 1971.
- [2] E. E. Baroody, C. Gotzmer, H. G. Adolph, *Energetic Melt Cast Explosives*, US Patent 5949016, September 7th 1999.
- [3] *EOD Information for Solid and Liquid Propellants, Conventional Explosives, and Other Dangerous Materials (U)*, Department of the Army Technical Manual, TM 9-1385-211, Headquarters, Department of the Army, January 1969.

## Bis(2,2-dinitropropyl)nitramine

Name [German, acronym]: Bis(dinitropropyl)nitramine [bis(2,2-dinitropropyl)nitramin, BDNPN]

Main (potential) use: Been investigated as possible RDX replacement, energetic additive<sup>[1]</sup>

Structural formula:



	<b>BDNPN</b>		
Formula	$C_6H_{10}N_6O_{10}$		
Molecular mass [g mol <sup>-1</sup> ]	326.18		
Appearance at RT			
IS [J]	>100 cm (ERL) <sup>[1]</sup>		
ESD [J]	>0.25 <sup>[1]</sup>		
N [%]	25.77		
$\Omega(CO_2)$ [%]	-34.3		
$T_{m.p.}$ [°C]			
$T_{dec.}$ [°C]			
$\rho$ [g cm <sup>-3</sup> ]	1.72 <sup>[1]</sup>		
Heat of formation	-230.12 kJ/mol ( $H_f$ ) <sup>[1]</sup>		
Impetus, force	1,295 J g <sup>-1</sup>		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{ex}U^\circ$ [kJ kg <sup>-1</sup> ]			
$T_{ex}$ [K]			
$p_{CJ}$ [kbar]			
VoD [m s <sup>-1</sup> ]			
$V_0$ [L kg <sup>-1</sup> ]			

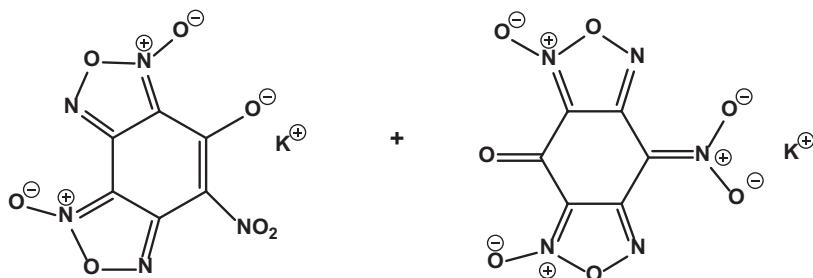
[1] E. Rozumov, T. Manning, D. Park, J. O'Reilly, *BDNPN as an Energetic Additive for Propellant Formulations*, ICT 2010, Karlsruhe, Germany, pp. 11-1-11-11.

## Bis(furoxano)nitrophenol, potassium salt

Name [German, acronym]: Potassium salt of bis(furoxano)nitrophenol, [bis(furoxano)nitrophenol kalium salz, KBFNP]

Main (potential) use: Possible candidate to replace LS<sup>[1,2,3]</sup>, may find applications in actuator or micro-propulsion systems<sup>[3]</sup>

Structural formula:<sup>†</sup>



<sup>†</sup> KBFNP is obtained as a mixture of two isomeric ring systems: *cis* (left) and *trans* (right)<sup>[3]</sup>

	KBFNP		
Formula	C <sub>6</sub> KN <sub>5</sub> O <sub>7</sub>		
Molecular mass [g mol <sup>-1</sup> ]	293.19		
Appearance at RT			
IS [J]	9 × 10 <sup>-3</sup> <sup>[1]</sup> , 0.009 ± 0.002 (ball drop apparatus) <sup>[2]</sup> , 0.009 ± 0.002 (ball drop apparatus, 62 °F, RH = 32%, sample predried @ 65 °C for >2 h) <sup>[3]</sup>		
FS [N]	No fire @ 20 g, low fire @ 30 g (BAM) <sup>[2]</sup> , no fire @ 20 g, low fire @ 30 g (69 °F, RH = 28%, small BAM method) <sup>[3]</sup>		
N [%]	23.89		
Ω(CO <sub>2</sub> ) [%]			
T <sub>m.p.</sub> [°C]			
T <sub>dec.</sub> [°C]	203 (DSC) <sup>[1]</sup> , 203 (exo, onset), 209 (exo, peak max.) (DSC @ 20 °C/min) <sup>[2,3]</sup>		
ρ [g cm <sup>-3</sup> ]	2.11 <sup>[1,3]</sup> , 2.07 <sup>[2]</sup>		
Heat of formation			
	Calcd. (EXPL05 6.04)	Lit. values	Exptl.

$-\Delta_{\text{ex}}U^\circ \text{ [kJ kg}^{-1}\text{]}$			
$T_{\text{ex}} \text{ [K]}$			
$p_{\text{C-J}} \text{ [kbar]}$			
$\text{VoD} \text{ [m s}^{-1}\text{]}$			
$V_0 \text{ [L kg}^{-1}\text{]}$			
Thermal stability	Stable @ 100 °C for extended periods of time but unstable @ higher temperatures <sup>[1]</sup> , 0.6% mass loss after 9,000 min @ 100 °C (TGA) <sup>[3]</sup> , 2.7% mass loss after 1,073 min and 34.7% mass loss after 5,400 min @ 120 °C <sup>[3]</sup>		
Witness plate tests	Average dent = 0.8 mils (cf. 37.3 mils for LA) (10 kpsi loading pressure in cavity, Al witness block, initiating charge (Zr/KClO <sub>4</sub> pyrotechnics)) <sup>[1]</sup> , average dent = 0.8 mils with charge density = 1.440 g cm <sup>-3</sup> (10.0 kpsi loading pressure, 200 mg sample, Al witness block) <sup>[2]</sup> , 10 kpsi loading pressure, 1.626 g cm <sup>-3</sup> average charge density, 0.80 mils average dent <sup>[3]</sup>		
Closed bomb test	$T_o - T_p = 0.501(0.003)$ ms, $T_o - T_{pk} = 0.670(0.017)$ ms, $T_{po} - T_{pk} = 0.169(0.016)$ ms, ignition time = 0.450(0.003) ms, peak pressure = 1499 psi, charge weight = 0.143 g, impetus = 6394 in lb/g (10 cc bomb, 15 kpsi loading pressure for KBFNP, initiated directly off a stainless steel 1-0 bridgewire with a 5A, 10 ms pulse, $T_o$ = application of pulse, $T_{po}$ = time to first indication of pressure, $T_{pk}$ = time to peak pressure) <sup>[3]</sup>		

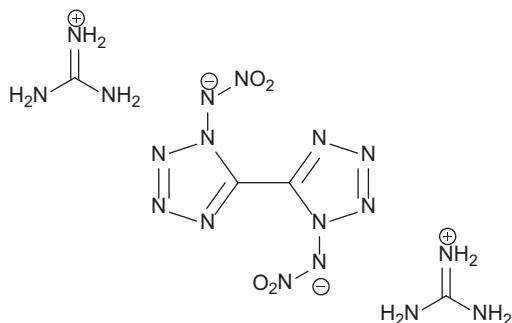
- [1] L. Türker, S. Varis, *A Review of Polycyclic Aromatic Energetic Materials*, in *Polycyclic Aromatic Compounds*, 2009, 29, 228–266.
- [2] M. Bichay, J. Hirlinger, *New Primary Explosives For Medium Caliber Stab Detonators*, SERDP Final Report, 1st September 2004.
- [3] J. W. Fronabarger, M. D. Williams, W. B. Sanborn, M. E. Sitzmann, M. Bichay, *Characterization and Output Testing of the Novel Primary Explosive, Bis(furoxano)nitrophenol, Potassium Salt*, 41st AIAA/ASME/SAE/ASEE Joint Propulsion Conference and Exhibit, 10–13th July 2005, Tucson, Arizona, USA.

## Bis(guanidinium) 1,1'-dinitramino-5,5'-bitetrazolate

Name [acronym]: Bis(guanidinium) 1,1'-dinitramino-5,5'-bitetrazolate  
[G2DNABT]

Main (potential) use: Secondary (primary) explosive

Structural formula:



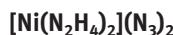
	G2DNABT
Formula	C <sub>4</sub> H <sub>12</sub> N <sub>18</sub> O <sub>4</sub>
Molecular mass [g mol <sup>-1</sup> ]	376.32
Appearance at RT	
IS [J]	4.9
FS [N]	120
N[%]	66.9
Ω(CO <sub>2</sub> ) [%]	-42.5
T <sub>dec.</sub> [°C]	210.5 (DSC @ 5 °C/min)
ρ [g cm <sup>-3</sup> ]	1.62 (@ 298 K)
Heat of formation	671.5 kJ/mol (ΔH <sup>o</sup> <sub>f</sub> )
	Calcd.
	Exptl.
– Δ <sub>ex</sub> U <sup>o</sup> [kJ kg <sup>-1</sup> ]	4,351
T <sub>ex</sub> [K]	
p <sub>CJ</sub> [kbar]	246
VoD [m s <sup>-1</sup> ]	7,693 (@ TMD)
V <sub>0</sub> [L kg <sup>-1</sup> ]	

## Bis-hydrazinenickel(II) azide

Name [German, acronym]: Hydrazine nickel azide [bis-hydrazinenickel(II) azid]

Main (potential) use: Possible Pb-free replacement for LA in primers<sup>[1]</sup>

Structural formula:



	<b>Bis-hydrazinenickel(II) azide</b>		
Formula	H <sub>8</sub> N <sub>10</sub> Ni		
Molecular mass [g mol <sup>-1</sup> ]	206.83		
Appearance at RT	Green-colored crystal aggregates <sup>[1]</sup>		
IS [J]	55 cm (10 kg mass) <sup>[1]</sup> , 10 cm (ball drop method, 500 g steel ball, height for 50% explosion) <sup>[2]</sup>		
FS [N]	Highly friction sensitive especially in dry state <sup>[2]</sup>		
N [%]	67.72		
Ω(CO <sub>2</sub> ) [%]			
T <sub>m.p.</sub> [°C]			
T <sub>dec.</sub> [°C]	186 (onset, DTA-TG) <sup>[1]</sup> , 196 (DTA @ 10 °C/min, air, 10 mg sample) <sup>[2]</sup>		
ρ [g cm <sup>-3</sup> ]	2.12 (crystal) <sup>[1]</sup>		
Heat of formation			
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
– Δ <sub>ex</sub> U° [kJ kg <sup>-1</sup> ]			
T <sub>ex</sub> [K]			
p <sub>C,J</sub> [kbar]			
VoD [m s <sup>-1</sup> ]			5,420 (@ 1.497 g cm <sup>-3</sup> ) <sup>[1]</sup>
V <sub>0</sub> [L kg <sup>-1</sup> ]			
Initiation efficiency	0.045 g (minimal charge in no. 8 detonator towards RDX) <sup>[1]</sup>		
5 s explosion T [°C] 5 s ignition T [°C]	~193 <sup>[1]</sup>		

Solubility [g/mL]	Insoluble in H <sub>2</sub> O, EtOH, Et <sub>2</sub> O <sup>[1]</sup>
Hygroscopicity	Nonhygroscopic <sup>[1]</sup>
Compatibility	Readily decomposed by acids and bases <sup>[1]</sup>

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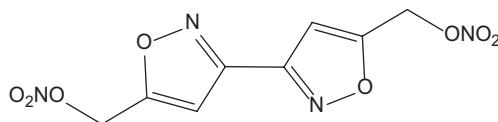
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## Bis-isoxazole-bis-methylene dinitrate

Name [German, acronym]: Bis-isoxazole-bis-methylene dinitrate, bis(isoxazole)-bis-(methylene) dinitrate, 3,3'-bis-isoxazole-5,5'-bis-methylene dinitrate [BIDN]

Main (potential) use: Potential new nitrate plasticizer and melt-castable secondary explosive<sup>[1,3]</sup>

Structural formula:



	<b>BIDN</b>		
Formula	C <sub>8</sub> H <sub>6</sub> N <sub>4</sub> O <sub>8</sub>		
Molecular mass [g mol <sup>-1</sup> ]	286.17		
Appearance at RT			
IS [J]	11.2 (modified P.A. apparatus) <sup>[1]</sup>		
FS [N]	>360 (BAM) <sup>[1]</sup>		
ESD [J]	0.250 (ABL machine) <sup>[1]</sup>		
N [%]	19.58		
Ω(CO <sub>2</sub> ) [%]	-61.5		
T <sub>m,p.</sub> [°C]	92.0 (onset), 95.9 (peak) (DSC @ 5 °C/min) <sup>[1]</sup> , 96.2 <sup>[3]</sup>		
T <sub>dec.</sub> [°C]	189.2 (onset), 221.2 (peak) (DSC @ 5 °C/min) <sup>[1]</sup> , 192.7 (onset) <sup>[3]</sup>		
ρ [g cm <sup>-3</sup> ]	1.585 (crystal) <sup>[1]</sup>		
Heat of formation	-139 kJ/mol (ΔH <sup>o</sup> <sub>f</sub> ) <sup>[1]</sup>		
	Calcd. (EXPL05 6.04)	Lit. values	Exptl.
- Δ <sub>ex</sub> U <sup>o</sup> [kJ kg <sup>-1</sup> ]			
T <sub>ex</sub> [K]			
p <sub>C,J</sub> [kbar]		19.3 GPa (calcd., CHEETAH 7.0) <sup>[1]</sup>	
VoD [m s <sup>-1</sup> ]		7,060 (@ 1.585 g cm <sup>-3</sup> , calcd., CHEETAH 7.0) <sup>[1]</sup>	
V <sub>0</sub> [L kg <sup>-1</sup> ]			

	<b>BIDN<sup>[2]</sup></b>
Chemical formula	C <sub>8</sub> H <sub>6</sub> N <sub>4</sub> O <sub>8</sub>
Molecular weight [g mol <sup>-1</sup> ]	286.17
Crystal system	Monoclinic
Space group	P2 <sub>1</sub> /n (no. 14)
<i>a</i> [Å]	6.1917(5)
<i>b</i> [Å]	5.5299(5)
<i>c</i> [Å]	17.4769(12)
$\alpha$ [°]	90
$\beta$ [°]	99.233(7)
$\gamma$ [°]	90
<i>V</i> [Å <sup>3</sup> ]	590.65(8)
<i>Z</i>	2
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.609
<i>T</i> [K]	296.85

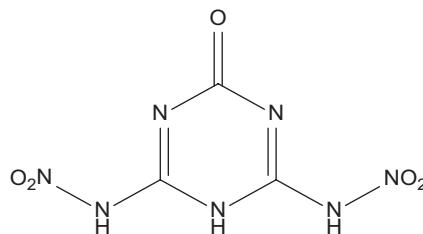
- [1] L. A. Wingard, P. E. Guzmán, E. C. Johnson, J. J. Sabatini, G. W. Drake, E. F. C. Byrd, *ChemPlusChem*, **2017**, *82*, 195–198.
- [2] R. C. Sausa, R. A. Pesce-Rodriguez, L. A. Wingard, P. E. Guzmán, J. J. Sabatini, *Acta Cryst.*, **2017**, *E73*, 644–646.
- [3] E. C. Johnson, J. J. Sabatini, D. E. Chavez, R. C. Sausa, E. F. C. Byrd, L. A. Wingard, P. E. Guzmán, *Org. Process Res. Dev.*, **2018**, *22*, 736–740.

## Bis(nitramino)triazinone

Name [German, acronym]: Bis(nitramino)triazinone [bis(nitramino)triazinon, 4,6-dinitroamino-1,3,5-triazine-2(1H)-one, DNAM]

Main (potential) use: Component of propellants<sup>[1]</sup>

Structural formula:



	<b>DNAM</b>		
Formula	C <sub>3</sub> H <sub>3</sub> N <sub>7</sub> O <sub>5</sub>		
Molecular mass [g mol <sup>-1</sup> ]	217.10		
Appearance at RT			
IS [J]	>50.5 (BAM) <sup>[1]</sup> , 82.5 Nm <sup>[2]</sup>		
FS [N]	216 <sup>[2]</sup> , >360 <sup>[1]</sup>		
ESD [J]	0.25 <sup>[2]</sup>		
N [%]	45.16		
Ω(CO <sub>2</sub> ) [%]	-18.4		
T <sub>m.p.</sub> [°C]	228 <sup>[6]</sup> , 228 (dec. without melting) <sup>[1]</sup>		
T <sub>dec.</sub> [°C]	228 <sup>[3]</sup>		
ρ [g cm <sup>-3</sup> ]	2.58 ± 0.1 (@ 293.15 K) <sup>[4,5]</sup> , 1.998 <sup>[2,6]</sup> , 1.949 (pycnometry) <sup>[1]</sup>		
Heat of formation	-111.21 kJ/mol (Δ <sup>o</sup> H <sub>f</sub> ) <sup>[1]</sup> , -111 kJ/mol (ΔH <sup>o</sup> <sub>f</sub> ) <sup>[2]</sup> , -512.25 kJ kg <sup>-1</sup> (ΔH <sup>o</sup> <sub>f</sub> ) <sup>[1]</sup>		
Heat of combustion	1,519.67 kJ/mol (Δ <sub>c</sub> H, measured) <sup>[1]</sup> , 1,508.11 kJ/mol (Δ <sub>c</sub> H, exptl. Parr bomb) <sup>[1]</sup>		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
- Δ <sub>ex</sub> U <sup>o</sup> [kJ kg <sup>-1</sup> ]			6,946.61 ± 68.13 <sup>[1]</sup>

$T_{\text{ex}}$ [K]		2,657 (@ 1.99 g cm <sup>-3</sup> , $\Delta H_f = -100$ kJ/mol, calcd., JAGUAR) <sup>[7]</sup>	
$p_{\text{C-J}}$ [GPa]		37.7 GPa (@ 1.99 g cm <sup>-3</sup> , $\Delta H_f = -100$ kJ/mol, calcd., JAGUAR) <sup>[7]</sup>	
VoD [m s <sup>-1</sup> ]		9,130 (@ 1.99 g cm <sup>-3</sup> , $\Delta H_f = -100$ kJ/mol, calcd., JAGUAR) <sup>[7]</sup>	9,200 <sup>[2]</sup>
$V_0$ [L kg <sup>-1</sup> ]			
Vacuum stability test [cm <sup>3</sup> /h]		0.257 cm <sup>3</sup> g <sup>-1</sup> after 40 h @ 100 °C <sup>[1]</sup>	

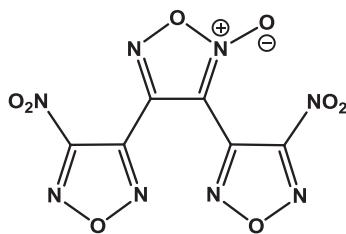
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- [2] R. Meyer, J. Köhler, A. Homburg, *Explosives*, 7th edn., Wiley-VCH, Weinheim, **2016**, pp. 32–33.
- [3] E. R. Atkinson, *J. Am. Chem. Soc.*, **1951**, *73*, 4443–4444.
- [4] Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994–2017 ACD/Labs).
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- [7] P. Samuels, K. Spangler, D. Iwaniuk, R. Cornell, E. L. Baker, L. I. Stiel, *Detonation Performance Analyses for recent Energetic Molecules*, AIP Conf. Proc., **1979**, 15003-1-150033-5.

## Bis(nitrofuranzano)furoxan

Name [German, acronym]: 3,4-Bis(4-nitro-1,2,5-oxadiazol-3-yl)-1,2,5-oxadiazole-N-oxide, 3,4-bis(4-nitro-1,2,5-oxadiazol-3-yl)-1,2,5-oxadiazole-N-oxide, 3,4-bis(4-nitro-1,2,5-oxadiazol-3-yl)-1,2,5-oxadiazole-2-oxide, 3,4-bis(3-nitrofurazan-4-yl)furoxan, 3,4-bis(4'-nitrofurazano-3'-yl)furoxan [BNFF, BNFF<sup>0</sup>, DNTF]

Main (potential) use: Possible future melt-castable explosive<sup>[3, 4]</sup>, possible ingredient in composite energetic formulations with improved stability<sup>[3]</sup>, possible future secondary explosive<sup>[3]</sup>, suggested as possible oxidizer for rocket propellant formulations<sup>[3]</sup>, possible energetic filler for propellants<sup>[4]</sup>, possible effective liquid-phase carrier in melt-cast explosives<sup>[9]</sup>

Structural formula:



\* The abbreviation BNFF<sup>0</sup> used for this compound by Zhang et al.<sup>[7]</sup> is used to distinguish it from BNFF (LLM-172, BNFF-1) in which the N-oxide group is not present. Unfortunately, in the literature BNFF has been used for DNTF and also for LLM-172.

	DNTF
Formula	C <sub>6</sub> N <sub>8</sub> O <sub>8</sub>
Molecular mass [g mol <sup>-1</sup> ]	312.1
Appearance at RT	White crystals <sup>[1]</sup> , colorless crystals <sup>[3]</sup> , white solid <sup>[9]</sup>
IS [J]	90% (cf. HMX = 100%, TNT = 4–6%; WL-1 type machine) <sup>[1]</sup> , $H_{50\%} = 0.31\text{ m}$ (type 12A tool, 2.5 kg mass, $35 \pm 2\text{ mg sample}$ , Bruceton method, type 12 ERL apparatus) <sup>[3]</sup> , <15.8 cm (ERL apparatus) <sup>[6]</sup> , >17 cm (2 kg mass, 30 mg sample, ZBL-B apparatus) <sup>[7]</sup> , $H_{50} = 25.9 \pm 0.08\text{ cm}$ (2–3 $\mu\text{m}$ , 2.5 kg mass, $35 \pm 1\text{ mg sample}$ , RT, ERL apparatus) <sup>[8]</sup> , $H_{50} = 25.3 \pm 0.06\text{ cm}$ (2–3 $\mu\text{m}$ , 2.5 kg mass, $35 \pm 1\text{ mg sample}$ , RT, ERL apparatus) <sup>[8]</sup> , $H_{50} = 25.1 \pm 0.07\text{ cm}$ (15–20 $\mu\text{m}$ , 2.5 kg mass, $35 \pm 1\text{ mg sample}$ , RT, ERL apparatus) <sup>[8]</sup> , $H_{50} = 24.9 \pm 0.08\text{ cm}$ (15–20 $\mu\text{m}$ , 2.5 kg mass, $35 \pm 1\text{ mg sample}$ , RT, ERL apparatus) <sup>[8]</sup> , 80–96% (10 kg, 25 cm) <sup>[9]</sup> , $H_{50} = 38.9\text{ cm}$ <sup>[9]</sup> , Navy method: ~17 cm (premelt), <8 cm –(postmelt) <sup>[6]</sup>

FS [N]	100% (cf. HMX = 100%, TNT = 4–6 %; WM-1 type machine) <sup>[1]</sup> , 120 (BAM high-friction sensitivity tester, porcelain pin and plate) <sup>[3]</sup> , >64 (BAM) <sup>[6]</sup> , 44% (swing angle = 90 °, 0.6 MPa gauge pressure, 30 mg sample, MGY-2 apparatus) <sup>[7]</sup> , $P = 13\%$ (2–3 µm, swing friction sensitivity tester, GJB-772) <sup>[8]</sup> , $P = 12\%$ (15–20 µm, swing friction sensitivity tester, GJB-772) <sup>[8]</sup> , 44–60% (90 °) <sup>[9]</sup>		
ESD [J]	>0.25 <sup>[6]</sup>		
N [%]	35.90		
$\Omega(\text{CO}_2)$ [%]	–20.5		
$T_{\text{m.p.}}$ [°C]	108.6–110.0 <sup>[1]</sup> , 109–111 <sup>[2]</sup> , 110 <sup>[3]</sup> , 109.0 (Mel-Temp apparatus, uncorrected) <sup>[3]</sup> , ~108 <sup>[6]</sup> , 109.43 (DSC @ 5 °C/min) <sup>[6]</sup> , 109–110 <sup>[7,9]</sup> , 108.9–109.6 (depends on heating rate used, DSC @ 1, 2, 5 or 10 K/min) <sup>[8]</sup> , 109.1 (DSC) <sup>[9]</sup> , 109.15 (DSC @ 0.1 MPa) <sup>[9]</sup> , 109.48 (DSC @ 2 MPa) <sup>[9]</sup> , 109.48 (DSC @ 4 MPa) <sup>[9]</sup> , 110.16 (DSC @ 6 MPa) <sup>[9]</sup>		
$T_{\text{dec.}}$ [°C]	292 (first stage dec.; second stage dec. @ 310 °C) <sup>[2]</sup> , 247.50 (exo onset), 273.71 (exo peak max) (DSC @ 5 °C/min) <sup>[6]</sup> , 248.48 (exo peak max, DSC @ 1 K/min) <sup>[8]</sup> , 256.52 (exo peak max, DSC @ 2 K/ min) <sup>[8]</sup> , 265.36 (exo peak max, DSC @ 5 K/min) <sup>[8]</sup> , 276.78 (exo peak max, DSC @ 10 K/min) <sup>[8]</sup> , 253.56 (exo peak max., DSC @ 0.1 MPa) <sup>[9]</sup> , 276.89 (DSC @ 2 MPa) <sup>[9]</sup> , 277.57 (DSC @ 4 MPa) <sup>[9]</sup> , 276.89 (DSC @ 6 MPa) <sup>[9]</sup> , 150 (weight loss begins, max. weight loss @ 212.18 °C, TG @ 10 °C/min, N <sub>2</sub> ) <sup>[9]</sup>		
$\rho$ [g cm <sup>−3</sup> ]	1.875 (@ RT) <sup>[2]</sup> , 1.937 <sup>[3,9]</sup> , 1.95 (calcd.) <sup>[6]</sup> , 1.93 <sup>[7]</sup>		
Heat of formation	657.23 (exptl.) <sup>[2]</sup> , 657.23 kJ/mol ( $\Delta_f H^\circ$ ) <sup>[4]</sup>		
Heat of combustion	9,733.96 J/g (in oxygen) <sup>[4]</sup> , 11,458 J/g <sup>[9]</sup>		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
– $\Delta_{\text{ex}} U^\circ$ [kJ kg <sup>−1</sup> ]		2,517 cal/cc (calcd.) <sup>[6]</sup>  5,789 J/g (@ 1.83 g cm <sup>−3</sup> ) <sup>[9]</sup>	5,797 <sup>[2]</sup>  5,795 (@ 1.86 g cm <sup>−3</sup> (heat of explosion)) <sup>[4]</sup>
$T_{\text{ex}}$ [K]		5,487 (@ 1.875 g cm <sup>−3</sup> , $\Delta H_f = 657$ kJ/mol, calcd., JAGUAR) <sup>[5]</sup>	
$p_{\text{CJ}}$ [kbar]		457.7 (@ 1.931 g cm <sup>−3</sup> , calcd. BKW) <sup>[1]</sup>  40.1 GPa (@ 1.875 g cm <sup>−3</sup> , $\Delta H_f = 657$ kJ/mol, calcd., JAGUAR) <sup>[5]</sup>	

		35.9 GPa (calcd.) <sup>[6]</sup> 41.1 GPa ( $\rho$ not specified) <sup>[7]</sup> 41.1 GPa (@ 1.937 g cm <sup>-3</sup> , calcd., VLW) <sup>[9]</sup>																																	
VoD [m s <sup>-1</sup> ]		9,250 (@ 1.931 g cm <sup>-3</sup> , calcd. BKW) <sup>[1]</sup> 9,050 (@ 1.875 g cm <sup>-3</sup> , $\Delta H_f = 657$ kJ/mol, calcd., JAGUAR) <sup>[5]</sup> 8,930 ( $\rho$ not specified) <sup>[7]</sup> 9,250 (@ 1.937, calcd., @ TMD) <sup>[8]</sup> 8,930 (@ 1.870 g cm <sup>-3</sup> ) <sup>[9]</sup>	8,930 <sup>[2]</sup> 8,930 (@ 1.86 g cm <sup>-3</sup> ) <sup>[4,5,9]</sup> 8,838 ± 13 (@ 1.847 g cm <sup>-3</sup> ) <sup>[9]</sup>																																
$V_0$ [L kg <sup>-1</sup> ]																																			
Power [% TNT]	172.4 (estimated by Berthelot's empirical equation) <sup>[1]</sup>																																		
5 s explosion $T$ [°C]	308 <sup>[1,4]</sup> , 315–340 <sup>[9]</sup>																																		
Thermal stability	Similar to that of HMX <sup>[4]</sup>																																		
Vacuum stability test [cm <sup>3</sup> /h]	0.45 mL gas/g @ 100 °C/48 h <sup>[4]</sup>	<p>The graph plots the volume of decomposition gases (cm<sup>3</sup>/g) on the y-axis (0 to 500) against time in minutes on the x-axis (0 to 5,000). Three data series are shown, each fitted with a solid line representing a first-order reaction description. The curves are labeled with their respective temperatures: 230 °C (top), 210 °C (middle), and 200 °C (bottom). All curves start at (0,0) and show an initial rapid increase in gas volume, which then levels off over time.</p> <table border="1"> <caption>Estimated data points from Figure 2</caption> <thead> <tr> <th>Time (min)</th> <th>200 °C (cm<sup>3</sup>/g)</th> <th>210 °C (cm<sup>3</sup>/g)</th> <th>230 °C (cm<sup>3</sup>/g)</th> </tr> </thead> <tbody> <tr><td>0</td><td>0</td><td>0</td><td>0</td></tr> <tr><td>500</td><td>~150</td><td>~250</td><td>~350</td></tr> <tr><td>1,000</td><td>~250</td><td>~350</td><td>~450</td></tr> <tr><td>2,000</td><td>~300</td><td>~400</td><td>~480</td></tr> <tr><td>3,000</td><td>~320</td><td>~420</td><td>~490</td></tr> <tr><td>4,000</td><td>~350</td><td>~450</td><td>~500</td></tr> <tr><td>5,000</td><td>~380</td><td>~480</td><td>~520</td></tr> </tbody> </table>		Time (min)	200 °C (cm <sup>3</sup> /g)	210 °C (cm <sup>3</sup> /g)	230 °C (cm <sup>3</sup> /g)	0	0	0	0	500	~150	~250	~350	1,000	~250	~350	~450	2,000	~300	~400	~480	3,000	~320	~420	~490	4,000	~350	~450	~500	5,000	~380	~480	~520
Time (min)	200 °C (cm <sup>3</sup> /g)	210 °C (cm <sup>3</sup> /g)	230 °C (cm <sup>3</sup> /g)																																
0	0	0	0																																
500	~150	~250	~350																																
1,000	~250	~350	~450																																
2,000	~300	~400	~480																																
3,000	~320	~420	~490																																
4,000	~350	~450	~500																																
5,000	~380	~480	~520																																

**Fig. 2:** Curves of the gas release during decomposition of DNTF at different temperatures ( $m/V \approx 10^{-3}$  g/cm<sup>3</sup>). Lines are the first-order reaction description<sup>[4]</sup>.

	(Manometric experiments, thin-walled glass manometer compensation type – the glass Bourdon gage @ 200–240 °C, 10–15 mg sample loaded in 12–15 cm <sup>3</sup> glass manometer, evacuated to 13.3 Pa, sealed and immersed in a thermostat in Wood's metal bath. The pressure of the gases evolved was converted into the gas volume at standard temperature and pressure) <sup>[4]</sup>  1.09 mL (5 g, 100 °C, 40 h) <sup>[9]</sup> , 1.88 mL (5 g, 120 °C, 20 h) <sup>[9]</sup>																																																																																	
Vapor pressure [atm. @ °C]	Dependence of vapor $p$ on $T$ : $\ln(p) = -8,321/T + 25.08$ <sup>[4]</sup>																																																																																	
Volatility	More volatile than RDX @ $T < 320$ °C but less volatile than RDX @ $T > 320$ °C <sup>[4]</sup> , vapor pressure above liq. DNTF is 3–7 times lower than the vapor pressure above TNAZ <sup>[4]</sup>																																																																																	
Burn rate [mm/s]	Similar to that of CL-20 <sup>[4]</sup> , samples pressed into 4 mm acrylic tubes ( $\rho = 1.75\text{--}1.76 \text{ g cm}^{-3}$ (93–94% TMD)) can sustain stable burning @ $p > 0.2 \text{ MPa}$ <sup>[4]</sup> , combustion @ atmospheric pressure is unstable <sup>[4]</sup> , burns with bright crimson flame @ $p > 3 \text{ MPa}$ <sup>[4]</sup>  ~1.3 mm/s @ 0.2 MPa <sup>[4]</sup> , ~1.8 mm/s @ 0.3 MPa <sup>[4]</sup> , 2 mm/s @ 0.5 MPa <sup>[4]</sup> , ~5 mm/s @ 1 MPa <sup>[4]</sup> , 10 mm/s @ 2.0 MPa <sup>[4]</sup> , ~20 mm/s @ 4.0 MPa <sup>[4]</sup> , ~25 mm/s @ 10.0 MPa <sup>[4]</sup> (samples as pressed plates, 10 mm long, 2 mm wide @ 1–1.5 mm thick) <sup>[4]</sup>  Burning rate-pressure dependence, $r_b = 5.6 \rho^{0.798} \text{ mm s}^{-1}$ for the pressure interval 0.2–15 MPa <sup>[4]</sup>																																																																																	
Solubility [g/mL]	Soluble in acetone ( $\geq 1.0 \text{ g in 10 mL}$ ) <sup>[1]</sup> , recryst. from isopropanol <sup>[3]</sup> , soluble in acetone, acetic acid, EtOH <sup>[9]</sup> , insoluble in water <sup>[9]</sup>  Exptl. mole fraction solubility values, $x_1$ of DNTF in pure EtOH and water binary system at saturation temperature $T_{\text{sat}}$ and pressure $P = 0.1 \text{ MPa}$ <sup>[10]</sup> :																																																																																	
<table border="1" style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th><math>x_2</math></th> <th><math>T_{\text{sat}}/\text{K}</math></th> <th><math>10^3 x_1</math></th> <th><math>x_2</math></th> <th><math>T_{\text{sat}}/\text{K}</math></th> <th><math>10^3 x_1</math></th> </tr> </thead> <tbody> <tr> <td>1.00</td> <td>312.55</td> <td>13.16</td> <td>0.85</td> <td>307.55</td> <td>5.74</td> </tr> <tr> <td></td> <td>317.15</td> <td>15.55</td> <td></td> <td>314.75</td> <td>7.96</td> </tr> <tr> <td></td> <td>322.55</td> <td>18.77</td> <td></td> <td>321.35</td> <td>10.59</td> </tr> <tr> <td></td> <td>328.55</td> <td>22.95</td> <td></td> <td>325.25</td> <td>12.44</td> </tr> <tr> <td></td> <td>334.25</td> <td>27.60</td> <td></td> <td>330.85</td> <td>15.63</td> </tr> <tr> <td></td> <td>340.95</td> <td>34.13</td> <td></td> <td>339.35</td> <td>21.74</td> </tr> <tr> <td>0.74</td> <td>308.35</td> <td>3.10</td> <td>0.64</td> <td>309.65</td> <td>1.94</td> </tr> <tr> <td></td> <td>315.95</td> <td>4.59</td> <td></td> <td>314.85</td> <td>2.58</td> </tr> <tr> <td></td> <td>323.05</td> <td>6.50</td> <td></td> <td>321.65</td> <td>3.70</td> </tr> <tr> <td></td> <td>327.75</td> <td>8.12</td> <td></td> <td>327.85</td> <td>5.07</td> </tr> <tr> <td></td> <td>333.35</td> <td>10.50</td> <td></td> <td>333.85</td> <td>6.84</td> </tr> <tr> <td></td> <td>339.85</td> <td>14.01</td> <td></td> <td>339.45</td> <td>8.89</td> </tr> </tbody> </table>					$x_2$	$T_{\text{sat}}/\text{K}$	$10^3 x_1$	$x_2$	$T_{\text{sat}}/\text{K}$	$10^3 x_1$	1.00	312.55	13.16	0.85	307.55	5.74		317.15	15.55		314.75	7.96		322.55	18.77		321.35	10.59		328.55	22.95		325.25	12.44		334.25	27.60		330.85	15.63		340.95	34.13		339.35	21.74	0.74	308.35	3.10	0.64	309.65	1.94		315.95	4.59		314.85	2.58		323.05	6.50		321.65	3.70		327.75	8.12		327.85	5.07		333.35	10.50		333.85	6.84		339.85	14.01		339.45	8.89
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	0.55	312.85	1.39	0.48	316.05	1.14
		316.85	1.79		319.45	1.41
		323.05	2.59		324.05	1.86
		327.25	3.29		329.35	2.57
		332.35	4.40		333.95	3.34
		338.05	5.98		337.95	4.16
Hygroscopicity	Not hygroscopic <sup>[9]</sup>					
Compatibility	Compatibility evaluations (1:1 mass:mass physical mixtures, DSC @ 5 °C/min, negative deviations ≥10 °C indicate fail <sup>[6]</sup> ):					
Material	Neat material			Material mixed with DNTF		
	Mpt. (°C)	Exo onset (°C)	Exo peak (°C)	Mpt. (°C)	Exo onset (°C)	Exo peak (°C)
DNTF	107.5	230.2	270.7	107.5	230.2	270.7
RDX	203.6	205.6	227.9	106.6	204.6	227.2
HMX	187.2	276.3	264.2	108.1	239.3	260.1
NTO	n/a	262.3	273.4	108.2	253.9	257.9
TATB	n/a	366.56	373.8	108.4	234.6	267.8
DNAN	94.2	326.9	342.9	68.9	241.8	271.9
NQ	n/a	195.2	202.8	108.5	182.8	225.5
DNP	86.5	275.8	296.9	78.3/102.1	208.5	248.7
Might be compatible with RDX, HMX and TNT <sup>[9]</sup>						
Flame temperature [K]	≤2,700 °C (max. surface $T$ ) <sup>[4]</sup> , 3,537 °C (calcd. adiabatic flame $T$ ) <sup>[4]</sup> ,					
Heat of vaporization [kJ/mol]	69.0 (est.) <sup>[4]</sup> , 75.3 (calcd.) <sup>[4]</sup>					
$\Delta H_{\text{melt}}$ [J/g]	86.32 (DSC @ 5 °C/min) <sup>[6]</sup>					
Activation energy for dec. [kJ/mol]	188.96 (Kissinger) <sup>[8]</sup>					

	DNTF <sup>[1]</sup>	DNTF <sup>[3]</sup>	DNTF <sup>[3]</sup>
Chemical formula	C <sub>6</sub> N <sub>8</sub> O <sub>8</sub>	C <sub>6</sub> N <sub>8</sub> O <sub>8</sub>	C <sub>6</sub> N <sub>8</sub> O <sub>8</sub>
Molecular weight [g mol <sup>-1</sup> ]	312.14	312.14	312.14
Crystal system	Orthorhombic	Orthorhombic	Orthorhombic
Space group	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>
$a$ [Å]	6.794(3)	6.7062(8)	7.028

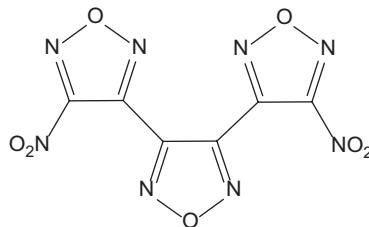
<i>b</i> [Å]	10.755(5)	10.7299(12)	11.212
<i>c</i> [Å]	15.137(5)	15.08308(17)	15.634
$\alpha$ [°]	90	90	90
$\beta$ [°]	90	90	90
$\gamma$ [°]	90	90	90
<i>V</i> [Å <sup>3</sup> ]	1,106.0(7)	1,085.3(2)	1,232.0
<i>Z</i>	4	4	
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.875	1.875	1.683
<i>T</i> [K]	293	150	
			Calculated values, MO6 method

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- [2] J. J. Sabatini, K. D. Oyler, *Crystals*, 2016, 6, 5.
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- [7] Y. Zhang, C. Zhou, B. Wang, Y. Zhou, K. Xu, S. Jia, F. Zhao, *Propellants, Explosives, Pyrotechnics*, 2014, 39, 809–814.
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- [9] Y. Zhou, B. Wang, J. Li, C. Zhou, L. Hu, Z. Chen, Z. Zhang, *Acta Chimica Sinica*, 2011, 69, 1673–1680.
- [10] L. Chen, L. Song, G. Lan, J. Wang, *Chinese J. Chem. Engineer.*, 2017, 25, 646–651.

## 3,4-Bis(4-nitro-1,2,5-oxadiazol-3-yl)-1,2,5-oxadiazole

Name [German, acronym]: Bis(nitrofuran)furazan<sup>[3]\*</sup> [3,4-bis(4-nitro-1,2,5-oxadiazol-3-yl)-1,2,5-oxadiazol, BNFF-1, LLM-172, BNFF<sup>[3]\*</sup>]

Main (potential) use: Possible new melt-castable secondary explosive<sup>[1,3]</sup>  
Structural formula:



\* The abbreviation BNFF used for this compound by Zhang et al.<sup>[3]</sup> is also used more commonly for DNTF which has a similar structure but with the addition of one N-oxide group. The compound 3,4-bis(4-nitro-1,2,5-oxadiazol-3-yl)-1,2,5-oxadiazole is more commonly abbreviated as BNFF-1 or LLM-172.

	BNFF-1
Formula	C <sub>6</sub> N <sub>8</sub> O <sub>7</sub>
Molecular mass [g mol <sup>-1</sup> ]	296.12
Appearance at RT	White very fine needles <sup>[3]</sup> , bright yellow crystal used for structure determination <sup>[3]</sup>
IS [J]	11.5 <sup>[1]</sup> , >25.1 (2 kg mass, 30 mg sample, ZBL-B apparatus) <sup>[3]</sup>
FS [N]	188 <sup>[1]</sup> , 8% (swing angle = 90 °, 0.6 MPa gauge pressure, 30 mg sample, MGY-2 apparatus) <sup>[3]</sup>
ESD [J]	>1.0 <sup>[1]</sup>
N [%]	37.84
Ω(CO <sub>2</sub> ) [%]	-27.0
T <sub>m.p.</sub> [°C]	85 <sup>[1]</sup> , 82.6 (endo, onset), 83.9 (endo, peak max) (DSC @ 10 °C/min) <sup>[3]</sup>
T <sub>phase transition</sub> [°C]	X-ray powder diffraction patterns show that on compression, the P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub> structure remains the predominant phase up to ~40 GPa <sup>[2]</sup>
T <sub>dec.</sub> [°C]	293 <sup>[1]</sup> , ~186.4 (exo, onset), 200.2 (exo, peak max) (DSC @ 10 °C/min) <sup>[3]</sup>
ρ [g cm <sup>-3</sup> ]	1.836 (crystalline) <sup>[1]</sup> , 1.839 (crystalline, @ 296 K) <sup>[3]</sup>
Heat of formation	644 kJ/mol (Δ <sub>f</sub> H <sup>o</sup> ) <sup>[1]</sup>

	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^{\circ}$ [kJ kg <sup>-1</sup> ]			
$T_{\text{ex}}$ [K]			
$p_{\text{CJ}}$ [kbar]		36.1 GPa ( $\rho$ not specified) <sup>[3]</sup>	
VoD [m s <sup>-1</sup> ]		8,680 ( $\rho$ not specified) <sup>[3]</sup>	
$V_0$ [L kg <sup>-1</sup> ]			
Solubility [g/mL]	Easily soluble in acetic acid, ethyl acetate, acetone, DMSO, DMF and conc. nitric acid <sup>[3]</sup> , some solubility in CH <sub>2</sub> Cl <sub>2</sub> , EtOH and MeOH <sup>[3]</sup> , and insoluble in water <sup>[3]</sup>		
Compatibility	Bleed gas method @ 100 °C, 40 h (0.5 g BNFF/0.5 g sample): 0.03 mL (sample = RDX), 0.05 mL (sample = HMX) and 0.08 mL (sample = TNT) therefore concluded that BNFF is compatible with RDX, HMX and TNT <sup>[3]</sup>		
$\Delta H_{\text{melt}}$ [J/g]	67.31 (DSC @ 10 °C/min) <sup>[3]</sup>		

	LLM-172 <sup>[2]</sup>	LLM-172 <sup>[2]</sup>	BNFF <sup>[3]</sup>
Chemical formula	C <sub>6</sub> N <sub>8</sub> O <sub>7</sub>	C <sub>6</sub> N <sub>8</sub> O <sub>7</sub>	C <sub>6</sub> N <sub>8</sub> O <sub>7</sub>
Molecular weight [g mol <sup>-1</sup> ]	296.14	296.14	296.14
Crystal system	Orthorhombic	Orthorhombic	Orthorhombic
Space group	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>
$a$ [Å]	7.1329(7)	7.125(2)	7.1493(10)
$b$ [Å]	9.6859(1)	9.575(8)	9.7887(14)
$c$ [Å]	15.1391(2)	15.080(6)	15.284(2)
$\alpha$ [°]	90	90	90
$\beta$ [°]	90	90	90
$\gamma$ [°]	90	90	90
$V$ [Å <sup>3</sup> ]	1,045.94	1,028.25	1,069.6(3)
$Z$	4		4
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]			1.839
$T$ [K]			296

	Single crystal	Powder X-ray diffraction @ ambient pressure and RT <sup>†</sup>	Single crystal, recryst. from EtOH
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<sup>†</sup>X-ray powder diffraction patterns show that on compression, the  $P2_12_12_1$  structure remains the predominant phase up to ~40 GPa<sup>[2]</sup>; LLM-172 remained semicrystalline up to 50 GPa under static compression<sup>[2]</sup>; increasing the pressure from ambient to 26 GPa results in a decrease in the volume of 35% (i.e., decreases of 3.8% in *a*-axis, 3.1% in *b*-axis and 6.2% in *c*-axis)<sup>[2]</sup>, at pressures >26 GPa only a 9% decrease was observed.<sup>[2]</sup>

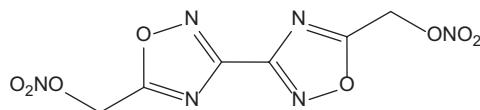
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- [3] Y. Zhang, C. Zhou, B. Wang, Y. Zhou, K. Xu, S. Jia, F. Zhao, *Propellants, Explosives, Pyrotechnics*, **2014**, *39*, 809–814.

## Bis(1,2,4-oxadiazole)bis(methylene)dinitrate

Name [German, acronym]: [3,3'-Bis(1,2,4-oxadiazole)]-5,5'-diylbis(methylene)dinitrate, [bis(1,2,4-oxadiazol)bis(methylen)dinitrat]

Main (potential) use: Potential new high-energy melt-castable explosive and energetic propellants plasticizing ingredient<sup>[1]</sup>

Structural formula:



	<b>Bis(1,2,4-oxadiazole)bis(methylene)dinitrate</b>		
Formula	C <sub>6</sub> H <sub>4</sub> N <sub>6</sub> O <sub>8</sub>		
Molecular mass [g mol <sup>-1</sup> ]	288.13		
Appearance at RT	White powder <sup>[1]</sup>		
IS [J]	8.7 <sup>[1]</sup>		
FS [N]	282 <sup>[1]</sup>		
ESD [J]	0.125 <sup>[1]</sup>		
N [%]	29.17		
Ω(CO <sub>2</sub> ) [%]	-33.3		
T <sub>m,p.</sub> [°C]	84.5 (DSC @ 5 °C/min) <sup>[1]</sup>		
T <sub>dec.</sub> [°C]	183.4 (onset), 214.6 (peak) (DSC @ 5 °C/min) <sup>[1]</sup>		
ρ [g cm <sup>-3</sup> ]	1.832 (crystal) <sup>[1]</sup>		
Heat of formation	-79.4 kJ/mol (Δ <sub>f</sub> H <sup>0</sup> ) <sup>[1]</sup>		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
- Δ <sub>ex</sub> U <sup>0</sup> [kJ kg <sup>-1</sup> ]			
T <sub>ex</sub> [K]			
p <sub>CJ</sub> [kbar]		29.4 GPa (@ 1.832 g cm <sup>-3</sup> , calcd.) <sup>[1]</sup>	
VoD [m s <sup>-1</sup> ]		8,180 (@ 1.832 g cm <sup>-3</sup> , calcd.) <sup>[1]</sup>	
V <sub>0</sub> [L kg <sup>-1</sup> ]			
I <sub>sp</sub> [s]	236.0 <sup>[1]</sup>		

	<b>Bis(1,2,4-oxadiazole)bis(methylene) dinitrate<sup>[1]</sup></b>
Chemical formula	C <sub>6</sub> H <sub>4</sub> N <sub>6</sub> O <sub>8</sub>
Molecular weight [g mol <sup>-1</sup> ]	288.15
Crystal system	Triclinic
Space group	P-1
a [Å]	4.8405(4)
b [Å]	6.0293(4)
c [Å]	9.4356(7)
α [°]	80.399(6)
β [°]	77.125(7)
γ [°]	78.831(6)
V [Å <sup>3</sup> ]	261.16(4)
Z	1
ρ <sub>calc</sub> [g cm <sup>-3</sup> ]	1.832
T [K]	295.9

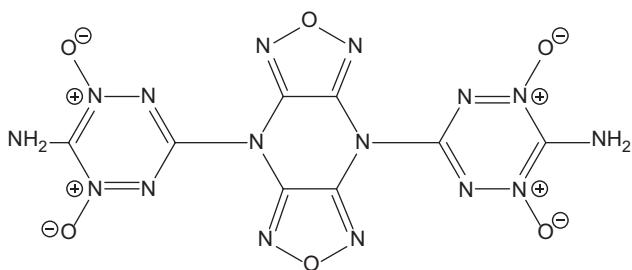
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**6,6'-(4*H*,8*H*-Bis[1,2,5]oxadiazolo[3,4-*b*:3',4'-*e*]pyrazine-4,8-diyi)bis(2,4-dioxo-1,2,4,5-tetrazin-3-amine)**

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

Main (potential) use: thermally stable explosive

Structural formula:



	<b>3,3'-(4<i>H</i>,8<i>H</i>-Bis([1,2,5]oxadiazolo)[3,4-<i>b</i>:3',4'-<i>e</i>]pyrazine-4,8-diyi)bis(6-amino-1,2,4,5-tetrazine 1,5-dioxide)</b>		
Formula	C <sub>8</sub> H <sub>4</sub> N <sub>16</sub> O <sub>6</sub>		
Molecular mass [g mol <sup>-1</sup> ]	420.23		
Appearance at RT	Clear yellow plate crystals (as DMF solvate) <sup>[1]</sup>		
IS [J]	$H_{50\%} = 18.5 \text{ cm}$ (LANL type 12, 2.5 kg mass) <sup>[1]</sup>		
FS [N]	>360 (50% load, Bruceton up/down method) <sup>[1]</sup>		
ESD [J]	0.062 (ABL spark, 3.4% threshold initiation level) <sup>[1]</sup>		
N [%]	53.33		
$\Omega(\text{CO}_2)$ [%]	-45.7		
T <sub>dec.</sub> [°C]	228 (onset), 275, 309 (DSC @ 10 °C/min, hermetically sealed Al pan) <sup>[1]</sup>		
$\rho$ [g cm <sup>-3</sup> ]	1.889 (calcd. @ 23 °C) <sup>[1]</sup> 1.66 1 (X-ray @ 150 K, DMF solvate) <sup>[1]</sup>		
Heat of formation	1,162 kJ/mol (enthalpy of form., calcd.) <sup>[1]</sup>		
	Calcd. (EXPL05 6.03)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^\circ$ [kJ kg <sup>-1</sup> ]			
T <sub>ex</sub> [K]			
p <sub>C-J</sub> [kbar]		33 GPa (@ 1.889 g cm <sup>-3</sup> , calcd., CHEETAH) <sup>[1]</sup>	

VoD [ $\text{m s}^{-1}$ ]		8,800 (@ 1.889 $\text{g cm}^{-3}$ , calcd., CHEETAH) <sup>[1]</sup>	
$V_0$ [ $\text{L kg}^{-1}$ ]			
$\Delta H_{\text{dec}}$ [J/g]	2,395 (DSC @ 10 °C/min, hermetically sealed Al pan) <sup>[1]</sup>		

	6,6'-(4H,8H-Bis[1,2,5]oxadiazolo[3,4-b:3',4'-e]pyrazine-4,8-diyl)bis(2,4-dioxo-1,2,4,5-tetrazin-3-amine) <i>N,N</i> -dimethylformamide solvate <sup>[1]</sup>
Chemical formula	$\text{C}_{8}\text{H}_{4}\text{N}_{16}\text{O}_6 \cdot 2\text{DMF}$
Molecular weight [g mol <sup>-1</sup> ]	566.46
Crystal system	Monoclinic
Space group	<i>C</i> 2/c
<i>a</i> [\mathring{A}]	11.8361(4)
<i>b</i> [\mathring{A}]	11.0288(4)
<i>c</i> [\mathring{A}]	17.3634(6)
$\alpha$ [°]	90
$\beta$ [°]	92.3283(10)
$\gamma$ [°]	90
<i>V</i> [\mathring{A} <sup>3</sup> ]	2264.71(14)
<i>Z</i>	4
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.661
<i>T</i> [K]	150

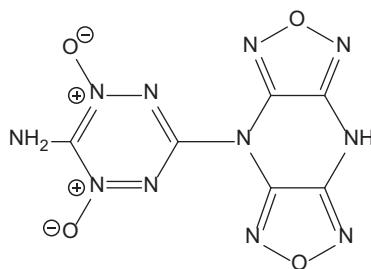
[1] C. J. Snyder, L. A. Wells, D. E. Chavez, G. H. Imler, D. A. Parrish, *Chem. Comm.*, **2019**, *55*, 2461–2464.

**6-(4*H*,8*H*-Bis[1,2,5]oxadiazolo[3,4-*b*:3',4'-3]pyrazine-4-yl)-2,4-dioxo-1,2,4,5-tetrazin-3-amine oxolan-2-one**

Name [German, acronym]: 6-Amino-3-(4*H*,8*H*-bis([1,2,5]oxadiazolo)[3,4-*b*:3',4'-*e*]pyrazin-4-yl)-1,2,4,5-tetrazine 1,5-dioxide

Main (potential) use: explosive

Structural formula:



	<b>6-Amino-3-(4<i>H</i>,8<i>H</i>-bis([1,2,5]oxadiazolo)[3,4-<i>b</i>:3',4'-<i>e</i>]pyrazin-4-yl)-1,2,4,5-tetrazine 1,5-dioxide</b>		
Formula	$C_6H_3N_{11}O_4$		
Molecular mass [g mol <sup>-1</sup> ]	293.16		
Appearance at RT	Clear yellow plate crystals (solvate) <sup>[1]</sup>		
IS [J]	$H_{50\%} \geq 78.4\text{ J}$ (LANL type 12, 2.5 kg mass) <sup>[1]</sup>		
FS [N]	>360 (50% load, Bruceton up/down method) <sup>[1]</sup>		
ESD [J]	0.062 (ABL spark, 3.4% threshold initiation level) <sup>[1]</sup>		
N [%]	52.56		
$\Omega(CO_2)$ [%]	-51.8		
$T_{dec.}$ [°C]	230 (exo, onset), 258 (exo, peak max) (DSC @ 10 °C/min, hermetically sealed Al pan) <sup>[1]</sup>		
$\rho$ [g cm <sup>-3</sup> ]	1.858 (calcd. @ 23 °C) <sup>[1]</sup>		
Heat of formation	810 kJ/mol (enthalpy of form., calcd.) <sup>[1]</sup>		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{ex}U^0$ [kJ kg <sup>-1</sup> ]			
$T_{ex}$ [K]			

$p_{C_J}$ [kbar]		32 GPa (@ 1.889 g cm <sup>-3</sup> , calcd., CHEETAH) <sup>[1]</sup>	
VoD [m s <sup>-1</sup> ]		8,400 (@ 1.889 g cm <sup>-3</sup> , calcd., CHEETAH) <sup>[1]</sup>	
$V_0$ [L kg <sup>-1</sup> ]			
$\Delta H_{dec}$ [J/g]	900 (DSC @ 10 °C/min, hermetically sealed Al pan) <sup>[1]</sup>		

	6-(4 <i>H</i> ,8 <i>H</i> -Bis[1,2,5]oxadiazolo[3,4- <i>b</i> :3',4'-3] pyrazine-4-yl)-2,4-dioxo-1,2,4,5-tetrazin-3- amine oxolan-2-one <sup>[1]</sup>
Chemical formula	C <sub>10</sub> H <sub>9</sub> N <sub>11</sub> O <sub>6</sub>
Molecular weight [g mol <sup>-1</sup> ]	379.28
Crystal system	Monoclinic
Space group	P2 <sub>1</sub> /n (no. 14)
<i>a</i> [Å]	5.5158(3)
<i>b</i> [Å]	9.6613(5)
<i>c</i> [Å]	27.7811(14)
$\alpha$ [°]	90
$\beta$ [°]	93.635(2)
$\gamma$ [°]	90
<i>V</i> [Å <sup>3</sup> ]	1,477.47(13)
<i>Z</i>	4
$\rho_{calc}$ [g cm <sup>-3</sup> ]	1.705
<i>T</i> [K]	293
	Solvate with γ-butyrolactone

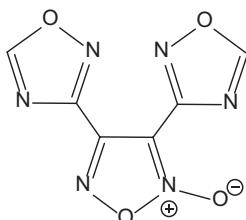
[1] C. J. Snyder, L. A. Wells, D. E. Chavez, G. H. Imler, D. A. Parrish, *Chem. Comm.*, **2019**, 55, 2461–2464.

## Bis(1,2,4-oxadiazolyl) furoxan

Name [German, acronym]: Bis(1,2,4-oxadiazolyl) furoxan

Main (potential) use: Promising melt-castable eutectic material with low sensitivity<sup>[1]</sup>

Structural formula:



	<b>Bis(1,2,4-oxadiazolyl) furoxan</b>		
Formula	$C_6H_2N_6O_4$		
Molecular mass [g mol <sup>-1</sup> ]	222.12		
Appearance at RT	Off-white solid <sup>[1]</sup>		
IS [J]	>34.7 <sup>[1]</sup>		
FS [N]	>360 <sup>[1]</sup>		
ESD [J]	>0.25 <sup>[1]</sup>		
N [%]	37.84		
$\Omega(CO_2)$ [%]	-64.9		
$T_{m.p.}$ [°C]	114.3 (onset, 117.8 °C peak max, DSC @ 5 °C/min) <sup>[1]</sup>		
$T_{dec.}$ [°C]	227 (onset, DSC @ 5 °C/min) <sup>[1]</sup>		
$\rho$ [g cm <sup>-3</sup> ]	1.79 (X-ray, @ 297 K) <sup>[1]</sup>		
Heat of formation	357 kJ/mol ( $\Delta H_f^\ominus$ ) <sup>[1]</sup>		
	Calcd. (EXPL05 6.03)	Lit. values	Exptl.
$-\Delta_{ex}U^\ominus$ [kJ kg <sup>-1</sup> ]			
$T_{ex}$ [K]			
$p_{C_J}$ [kbar]		24.1 GPa (calcd., Cheetah 7.0) <sup>[1]</sup>	
VoD [m s <sup>-1</sup> ]		7,577 (@ 1.70 g cm <sup>-3</sup> , calcd., CHEETAH 7.0) <sup>[1]</sup>	
$V_0$ [L kg <sup>-1</sup> ]			

	Bis(1,2,4-oxadiazolyl) furoxan <sup>[1]</sup>
Chemical formula	C <sub>6</sub> H <sub>2</sub> N <sub>6</sub> O <sub>4</sub>
Molecular weight [g mol <sup>-1</sup> ]	222.14
Crystal system	Monoclinic
Space group	P2 <sub>1</sub>
<i>a</i> [Å]	6.3295(17)
<i>b</i> [Å]	7.6697(8)
<i>c</i> [Å]	9.0120(14)
$\alpha$ [°]	90
$\beta$ [°]	109.63(2)
$\gamma$ [°]	90
<i>V</i> [Å <sup>3</sup> ]	412.07(15)
<i>Z</i>	2
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.790
<i>T</i> [K]	297

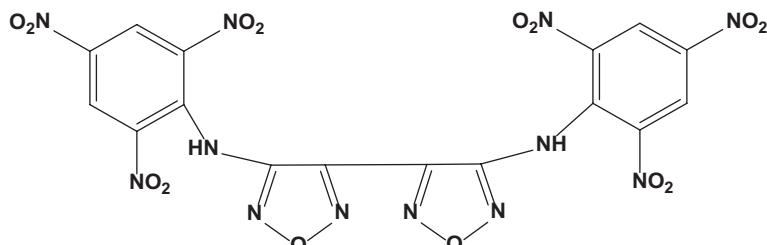
[1] E. C. Johnson, E. J. Bukowski, J. J. Sabatini, R. C. Sausa, E. F. C. Byrd, M. A. Garner, D. E. Chavez, *ChemPlusChem*, **2019**, 84, in press.

## 4,4'-Bis(picrylamino)-3,3'-bisfurazanyl

Name [German, acronym]: 4,4'-Bis(picrylamino)-3,3'-bisfurazanyl [BPABF]

Main (potential) use: Potential future thermally stable explosive<sup>[1,2]</sup>

Structural formula:



	<b>BPABF</b>		
Formula	C <sub>16</sub> H <sub>6</sub> N <sub>12</sub> O <sub>4</sub>		
Molecular mass [g mol <sup>-1</sup> ]	590.29		
Appearance at RT			
IS [J]	10 (BAM) <sup>[2]</sup>		
FS [N]	360 (BAM) <sup>[2]</sup>		
ESD [J]	0.75 (OZM apparatus) <sup>[2]</sup>		
N [%]	28.47		
Ω(CO <sub>2</sub> ) [%]	-13.5		
T <sub>dec.</sub> [°C]	320 (DTA @ 5 °C/min) <sup>[2]</sup>		
ρ [g cm <sup>-3</sup> ]	1.786 (crystal @ 173 K) <sup>[2]</sup>		
Heat of formation	506.5 kJ/mol (Δ <sub>f</sub> H°, calcd., atomization method, CBS-4M) <sup>[2]</sup>		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
- Δ <sub>ex</sub> U° [kJ kg <sup>-1</sup> ]	921.5 (@ 1.786 g cm <sup>-3</sup> , Δ <sub>f</sub> H° = 506.5 kJ/mol) <sup>[2]</sup>		
T <sub>ex</sub> [K]	3,661 (@ 1.786 g cm <sup>-3</sup> , Δ <sub>f</sub> H° = 506.5 kJ/mol) <sup>[2]</sup>		
p <sub>CJ</sub> [kbar]	248 (@ 1.786 g cm <sup>-3</sup> , Δ <sub>f</sub> H° = 506.5 kJ/mol) <sup>[2]</sup>		
VoD [m s <sup>-1</sup> ]	7,719 (@ 1.786 g cm <sup>-3</sup> , Δ <sub>f</sub> H° = 506.5 kJ/mol) <sup>[2]</sup>		
V <sub>0</sub> [L kg <sup>-1</sup> ]			

Vacuum stability test [cm <sup>3</sup> /h]	1.2 mL/g @ 120 °C, 40 h (0.2 g sample) <sup>[2]</sup>
Compatibility	(DTA @ 5 °C/min, BPABF mixed with equivalent wt.% of second compound): BPABF compatible with Cu, CuO, Al, RDX, TNT, DNAN and HTPB <sup>[2]</sup>

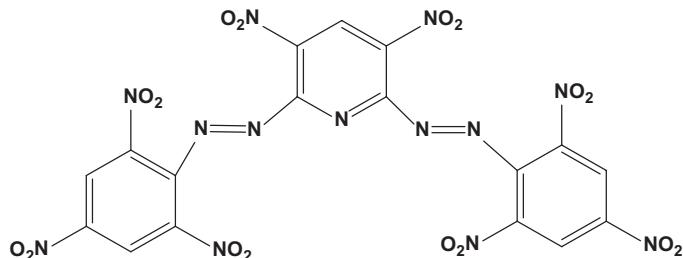
	<b>BPABF<sup>[2]</sup></b>
Chemical formula	C <sub>16</sub> H <sub>6</sub> N <sub>12</sub> O <sub>14</sub>
Molecular weight [g mol <sup>-1</sup> ]	590.33
Crystal system	Monoclinic
Space group	P2 <sub>1</sub> /c
a [Å]	31.7742(8)
b [Å]	8.1232(2)
c [Å]	8.5090(2)
α [°]	90
β [°]	91.957(7)
γ [°]	90
V [Å <sup>3</sup> ]	2,194.96
Z	4
ρ <sub>calc</sub> [g cm <sup>-3</sup> ]	1.78
T [K]	173

[1] S. R. Ahmad, M. Cartwright, *Laser Ignition of Energetic Materials*, John Wiley and Sons, 2014.

[2] T. Hermann, *Investigation of Oxygen- and Nitrogen-Rich Heterocyclic Compounds as Potential High-Energy Dense Oxidizers or Secondary Explosives*, PhD Thesis, Ludwig-Maximilian University, Munich, Germany, 2018.

### **2,6-Bis(picrylazo)-3,5-dinitropyridine**

Name [German, acronym]: Bis[picrylazo] dinitropyridine [PADP]  
Main (potential) use: Thermally stable detonator explosive<sup>[1]</sup>  
Structural formula:



$V_0$ [L kg <sup>-1</sup> ]			
Vacuum stability test [cm <sup>3</sup> /h]	@ 150 °C, total gas evolved (cm <sup>3</sup> /g) @ STP/time of exposure (days) <sup>[2]</sup> : 5.3/2, 4.9/7, 4.3/14, 4.1/21, 3.9/28, 4.1/35, 4.2/42, 4.2/49, 4.3/56, 4.4/63, 4.5/70, 4.7/77, 4.9/84, 5.0/91 <sup>[2]</sup>		

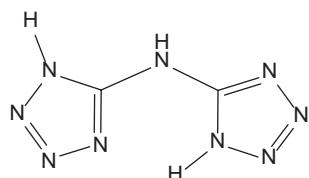
- [1] M. D. Coburn, B. W. Harris, K.-Y. Lee, M. M. Stinecipher, H. H. Hayden, *Ind. Eng. Chem. Prod. Res. Dev.*, **1986**, *25*, 68–72.
- [2] W. Yang, R. A. Parrott, L. A. Behrmann, W. E. Voreck, P. Kneisel, *High Temperature Explosives for Downhole Well Applications*, US Patent US 2002/0129940 A1, 19th September **2002**.
- [3] *LASL Explosive Property Data*, T. R. Gibbs, A. Popolato (eds.), University of California Press, Berkeley, **1980**.

## 5,5'-Bis(1*H*-tetrazolyl)amine

Name [German, acronym]: *N,N*-Bis(1(2)*H*-tetrazol-5-yl)amine, [5,5'-bis(1*H*-tetrazolyl)amin, H<sub>2</sub>BTA]

Main (potential) use: gas generant

Structural formula:



	<b>H<sub>2</sub>BTA</b>
Formula	C <sub>2</sub> H <sub>3</sub> N <sub>9</sub>
Molecular mass [g mol <sup>-1</sup> ]	155.13
Appearance at RT	
IS [J]	>30 (BAM) <sup>[1]</sup>
FS [N]	360 (BAM) <sup>[1]</sup>
ESD [J]	7.5 <sup>[1]</sup>
N [%]	-57.47 <sup>[1]</sup>
Ω(CO <sub>2</sub> ) [%]	82.34
T <sub>dec.</sub> [°C]	250 (DSC @ 5 °C/min, covered Al, N <sub>2</sub> ) <sup>[1]</sup> TG-DTG @ 10 °C/min <sup>[2]</sup> : 

Fig.3: TG-DTG curves of H<sub>2</sub>BTA at a heating rate of 10 °C/min<sup>[2]</sup>.

	DSC data at different heating rates <sup>[2]</sup> :			
$\beta$ (°C/min)	$T_{p2}$ (°C)	$T_{p3}$ (°C)	$\Delta H_d$ (J/g)	
5	261.03	270.09	636.22	
8	264.66	276.79	769.59	
10		279.14	797.34	
15		283.54	896.68	
20		285.42	1,001.6	
$\rho$ [g cm <sup>-3</sup> ]	1.861 (X-ray) <sup>[1]</sup> , 1.86 <sup>[2]</sup>			
Heat of formation	633 kJ/mol ( $\Delta H_f^\circ$ ) <sup>[1]</sup>			
Heat of combustion	-1,858 kJ/mol <sup>[1]</sup>			
	Calcd. (EXPLO5 5.02)	Lit. values	Exptl.	
- $\Delta_{ex} U^\circ$ [kJ kg <sup>-1</sup> ]	4537 <sup>[1]</sup>			
$T_{ex}$ [K]	3,449 <sup>[1]</sup>			
$p_{C,I}$ [kbar]	343 <sup>[1]</sup>			
VoD [m s <sup>-1</sup> ]	9,120 (@ 1.861 g cm <sup>-3</sup> ) <sup>[1]</sup>			
$V_0$ [L kg <sup>-1</sup> ]	753 <sup>[1]</sup>			
$\Delta H_{dec}$ [J/g]	636.22 (DSC @ 5 °C/min) <sup>[2]</sup> , 769.59 (DSC @ 8 °C/min) <sup>[2]</sup> , 797.34 (DSC @ 10 °C/min) <sup>[2]</sup> , 896.68 (DSC @ 15 °C/min) <sup>[2]</sup> , 1,001.6 (DSC @ 20 °C/min) <sup>[2]</sup>			
Koenen test	24.0 g sample destroyed steel tube into >10 fragments with 8 mm hole and also with 10 mm hole <sup>[1]</sup>			

	<b>H<sub>2</sub>BTA<sup>[1]</sup></b>
Chemical formula	C <sub>2</sub> H <sub>3</sub> N <sub>9</sub>
Molecular weight [g mol <sup>-1</sup> ]	153.13
Crystal system	Orthorhombic
Space group	Pbca (no. 61)
<i>a</i> [Å]	11.109(2)
<i>b</i> [Å]	9.227(2)
<i>c</i> [Å]	21.327(4)
$\alpha$ [°]	90

$\beta$ [°]	90
$\gamma$ [°]	90
$V$ [\AA <sup>3</sup> ]	2,186.1(7)
$Z$	16
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.861
$T$ [K]	200

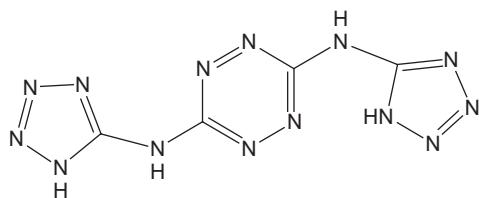
- [1] J. Stierstorfer, *Advanced Energetic Materials Based on 5-Aminotetrazole – Synthesis, Characterization and Scale-Up*, PhD Thesis, LMU München, Munich, **2009**.
- [2] L.-L. Wang, Y. Liu, S.-T. Zhao, *Chinese J. Explosives, Propellants*, **2018**, 41, 47–51.

## 3,6-Bis(1*H*-1,2,3,4-tetrazol-5-yl-amino)-*s*-tetrazine

Name [German, acronym]: 3,6-Bis(1*H*-1,2,3,4-tetrazol-5-yl-amino)-1,2,4,5-tetrazine,  
[3,6-bis(1*H*-1,2,3,4-tetrazol-5-yl-amino)-1,2,4,5-tetrazin,  
BTATz]

Main (potential) use: Patented as component of propellant compositions<sup>[2]</sup>,  
energetic fuel<sup>[2,4]</sup>, possible component of future  
solid propellants<sup>[3]</sup>, possible substitute for Al in  
propellants<sup>[4]</sup>, fire suppressant applications<sup>[7,10]</sup>,  
gas-generating ingredient in car airbags<sup>[7,10]</sup>,  
solid rocket motor propellant<sup>[10]</sup>

Structural formula:



	<b>BTATz</b>
Formula	C <sub>4</sub> H <sub>4</sub> N <sub>14</sub>
Molecular mass [g mol <sup>-1</sup> ]	248.17
Appearance at RT	Orange-brown powder <sup>[2,4]</sup> , orange crystals (recryst. from warm DMSO) <sup>[7]</sup> , rod-type crystals <sup>[7]</sup> , thin light orange plates <sup>[10]</sup> , reddish-brown solid <sup>[12]</sup>
IS [J]	7 <sup>[1]</sup> , 195 cm (type 12, cf. HMX = 24–27 cm) <sup>[2,11]</sup> , >32 cm (cf. HMX = 25 cm) <sup>[3]</sup> , H <sub>50</sub> = 40 cm <sup>[5]</sup> , H <sub>50%</sub> = 116 ± 5 cm (2 kg mass) <sup>[7]</sup> , H <sub>50</sub> = 32 cm (type 12 tool, 2.5 kg mass) <sup>[8]</sup> , DH <sub>50</sub> = 207 cm <sup>[10]</sup> , H <sub>50</sub> = 160–200 cm (2.5 kg mass) <sup>[12]</sup>
FS [N]	>360 <sup>[1]</sup> , >36 kg <sup>[5]</sup> , 36 ± 0.2 kg (Julius-Peters, 0/5 tests) <sup>[7]</sup>
ESD [J]	>0.36 <sup>[5]</sup> , 190 mJ <sup>[7]</sup>
N [%]	79.0
Ω(CO <sub>2</sub> ) [%]	-64.5
T <sub>m.p.</sub> [°C]	264 (dec., Mettler FPI apparatus @ 2 °C/min, corrected) <sup>[2,4]</sup> , 270 (dec.) <sup>[7]</sup> , 264 – 285 (DSC @ 10 °C/min) <sup>[12]</sup>
T <sub>b.p.</sub> [°C]	590 (est.) <sup>[8]</sup>

$T_{\text{dec.}}$ [°C]	264 (dec., Mettler FPI apparatus @ 2 °C/min, corrected) <sup>[2,4]</sup> , 264 (DSC, onset) <sup>[5]</sup> , 270 (dec.) <sup>[7]</sup> , $T_i = 265$ , $T_m = 320$ , $T_f = 350$ (DSC @ 10 °C/min) <sup>[7]</sup> , 93% mass loss @ 271–338 °C (TG) <sup>[7]</sup> , 579 K (DSC @ 5 °C/min) <sup>[7]</sup> , 588 K (DSC @ 10 °C/min) <sup>[7]</sup> , 593 K (DSC @ 15 °C/min) <sup>[7]</sup> , 597 K (DSC @ 20 °C/min) <sup>[7]</sup> , 264 (DSC), 320 (DSC), 306.8 (DSC @ 4 °C/min, pressed in Al caps, nonisothermal) <sup>[8]</sup> , 316.6 (DSC @ 8 °C/min, pressed in Al caps, nonisothermal) <sup>[8]</sup> , 323.7 (DSC @ 16 °C/min, pressed in Al caps, nonisothermal) <sup>[8]</sup> , 334.2 (DSC @ 32 °C/min, pressed in Al caps, nonisothermal) <sup>[8]</sup> , 317.12 (DSC @ 10 °C/min) <sup>[9]</sup> , 320.5 (onset), 338.9 (peak max) (DSC @ 10 °C/min) <sup>[10]</sup> , 320 (peak max, DSC @ 10 °C/min) <sup>[12]</sup>		
$\rho$ [g cm <sup>-3</sup> ]	1.74 <sup>[1]</sup> , 1.76 (gas pycnometry) <sup>[2,4,11]</sup> , 1.76 <sup>[6,8,12]</sup> , 1.742 <sup>[8]</sup> , 1.71 (pressed strand) <sup>[8]</sup> , 1.90 (@ 85 K) <sup>[10]</sup> , 1.78 (@ 298 K) <sup>[10]</sup>		
Heat of formation	3.55 kJ/g ( $\Delta H_f^\circ$ ) <sup>[1]</sup> , 883 kJ/mol ( $\Delta H_f^\circ$ ) <sup>[3,6,12]</sup> , 882.2 kJ/mol ( $\Delta H_f^\circ$ ) <sup>[8]</sup> , 711 kJ/mol ( $\Delta H_f^\circ$ ) <sup>[8]</sup> , 211 kcal/mol (measured) <sup>[11]</sup>		
Heat of combustion	12,204.13 kJ/mol <sup>[12]</sup>		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^\circ$ [kJ kg <sup>-1</sup> ]		3,557 (calcd., LOTUSES) <sup>[7]</sup>	
$T_{\text{ex}}$ [K]			
$p_{\text{CJ}}$ [kbar]		25.39 GPa (@ 1.78 g cm <sup>-3</sup> , calcd., CHEETAH 7.0) <sup>[10]</sup>	
VoD [m s <sup>-1</sup> ]		7,520 (@ 1.76 g cm <sup>-3</sup> , calcd.) <sup>[8]</sup>  8,055 (@ 1.78 g cm <sup>-3</sup> , calcd., CHEETAH 7.0) <sup>[10]</sup>  7,520 (@ 1.75 g cm <sup>-3</sup> , calcd.) <sup>[12]</sup>	
$V_0$ [L kg <sup>-1</sup> ]		1,237 (calcd., LOTUSES) <sup>[7]</sup>	
$I_s$ [s]	215 (BTATz as monopropellant) <sup>[2,4]</sup> , 232 (70 wt.% AP, ~14% HTPB, EPDI, DOA, 16% BTATz which is 88% of the performance of the corresponding Al-containing system (Al replaced BTATz)) <sup>[2,4]</sup> , $I_{\text{sp}}$ (calcd.) = 219 s (calcd., BKW EOS using CHEETAH 2.0 code @ 68.03 atm, 1 atm exit pressure) <sup>[5]</sup>		

Critical diameter [cm]	Pressed pellet of 0.5 in diameter does not detonate <sup>[2,4]</sup>																																																																						
Critical T [K]	585.30 (critical $T$ for thermal explosion) <sup>[6]</sup>																																																																						
Thermal stability	DSC, $T_{\text{SADT}}$ = self-accelerating decomposition temperature, $T_b$ = critical $T$ of thermal explosion, $T_{\text{ITT}}$ = thermal ignition temperature <sup>[6]</sup> : $T_{\text{SADT}} = 559.28 \text{ K}$ , $T_{\text{ITT}} = 572.76 \text{ K}$ , $T_b = 585.30 \text{ K}$ <sup>[6]</sup> , 93% mass loss @ 271–338 °C (TG) <sup>[7]</sup> , no self-accelerating dec. observed @ 250–285 °C, max. gas release = 280 cm <sup>3</sup> /g <sup>[8]</sup>  Approx. volume of dec. gases (cm <sup>3</sup> /g) @ various temperatures versus time (min) <sup>[8]</sup> :																																																																						
	<table border="1"> <thead> <tr> <th>Time (min)</th> <th colspan="4"><math>T</math> (°C)</th> </tr> <tr> <th></th> <th>250</th> <th>270</th> <th>280</th> <th>285</th> </tr> </thead> <tbody> <tr> <td>5</td> <td>0</td> <td>10</td> <td>10</td> <td>10</td> </tr> <tr> <td>25</td> <td>10</td> <td>40</td> <td>80</td> <td>80</td> </tr> <tr> <td>50</td> <td>20</td> <td>80</td> <td>200</td> <td>220</td> </tr> <tr> <td>75</td> <td>25</td> <td>110</td> <td>240</td> <td>—</td> </tr> <tr> <td>95</td> <td>30</td> <td>125</td> <td>245</td> <td>—</td> </tr> <tr> <td>100</td> <td>—</td> <td>130</td> <td>250</td> <td>—</td> </tr> <tr> <td>145</td> <td>50</td> <td>180</td> <td>260</td> <td>—</td> </tr> <tr> <td>195</td> <td>70</td> <td>220</td> <td>—</td> <td>—</td> </tr> <tr> <td>225</td> <td>75</td> <td>—</td> <td>—</td> <td>—</td> </tr> <tr> <td>255</td> <td>85</td> <td>—</td> <td>—</td> <td>—</td> </tr> <tr> <td>295</td> <td>95</td> <td>—</td> <td>—</td> <td>—</td> </tr> <tr> <td>325</td> <td>105</td> <td>—</td> <td>—</td> <td>—</td> </tr> </tbody> </table>	Time (min)	$T$ (°C)					250	270	280	285	5	0	10	10	10	25	10	40	80	80	50	20	80	200	220	75	25	110	240	—	95	30	125	245	—	100	—	130	250	—	145	50	180	260	—	195	70	220	—	—	225	75	—	—	—	255	85	—	—	—	295	95	—	—	—	325	105	—	—	—
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255	85	—	—	—																																																																			
295	95	—	—	—																																																																			
325	105	—	—	—																																																																			
Burn rate [mm/s]	BTATz/3% Kel-F: $I_{sp} = 219 \text{ s}$ , $\beta = 1.78 \text{ cm}\cdot\text{s}^{-1}\cdot\text{MPa}^\alpha$ , $\alpha = 0.49$ , range = 0.2 – 20 MPa <sup>[1]</sup> BTATz/3% Kel-F 800 (approx. values taken from graph, burn rate (cm/s) @ pressure (atm.)) <sup>[2,4]</sup> : 2.5 cm/s @ 0.7 atm, 5.5 cm/s @ 90 atm. <sup>[2,4]</sup> , 6 cm/s @ 150 atm. <sup>[2,4]</sup> BTATz/3% Kel-F: 0.55 cm/s @ 0.6 atm <sup>[3]</sup> , 1 cm/s @ 3 atm. <sup>[3]</sup> , 1.75 cm/s @ 15 atm. <sup>[3]</sup> , 3 cm/s @ 35 atm. <sup>[3]</sup> , 7 cm/s @ 100 atm. <sup>[3]</sup> 4.59 cm·s <sup>-1</sup> @ 68 atm. <sup>[5]</sup> , burning rate exponent = 0.49 <sup>[5]</sup> BTATz burns rapidly generating 0.7 L N <sub>2</sub> (g) per gram solid BTATz <sup>[7]</sup> , burns without producing smoke and produces minimal residue <sup>[7]</sup> , burns with minimal smoke <sup>[10]</sup>																																																																						

	Burning rates (mm/s) at different pressures (atm) with different BTATz samples <sup>[8]</sup> :			
Sample				
BTATz	BTATz from DMF	BTATz from EtOH	BTATz from EtOH	
4 @ 1 atm.	45 @ 7 atm.	20 @ 7 atm.	6 @ 1 atm.	
9 @ 2 atm.	70 @ 40 atm.	18 @ 15 atm.	45 @ 35 atm.	
10 @ 3 atm.	90 @ 100 atm.	31 @ 30 atm.	55 @ 70 atm.	
10 @ 4 atm.		55 @ 55 atm.	65 @ 120 atm.	
12 @ 5 atm.				
15 @ 6 atm.				
19 @ 11 atm.				
21 @ 20 atm.				
30 @ 40 atm.				
50 @ 70 atm.				
5.6 @ 0.1 MPa <sup>[12]</sup> , 75 @ 19 MPa <sup>[12]</sup>				
Solubility [g/mL]	Recryst. from DMSO/MeOH <sup>[2]</sup> , soluble in warm DMSO <sup>[2,7]</sup> , poor solubility in most common organic solvents <sup>[10]</sup> , insoluble in water, acetone, acetonitrile, DMF <sup>[12]</sup> , soluble in DMSO and hot benzene <sup>[12]</sup>			
$\Delta H_{\text{dec}}$ [J/g]	1562 (DSC @ 10 °C/min) <sup>[7]</sup> , 1339 (DSC, pressed in Al caps) <sup>[8]</sup>			
Flame test	Max. flame $T$ does not exceed 800 K <sup>[8]</sup>			
Surface $T$ [K]	520–665 °C (in pressure range studied) <sup>[8]</sup>			
Heat of vaporization [kJ/mol]	129.3 (est.) <sup>[8]</sup>			
Thermal diffusivity	$(6.0 \pm 0.3) \times 10^{-3} \text{ cm}^2 \text{s}^{-1}$ (molten BTATz in $T$ interval 300–650 °C) <sup>[8]</sup>			
Specific heat [J/g K]	1.67 (approx.) <sup>[8]</sup>			

	<b>BTATz<sup>[10]</sup></b>	<b>BTATz-DMF<sup>[10]</sup></b>	<b>BTATz-pyridine<sup>[10]</sup></b>	<b>BTATz-pyr-N-oxide<sup>[10]</sup></b>	<b>BTATz-2-pyridone<sup>[10]</sup></b>	<b>BTATz-pyrazine<sup>[10]</sup></b>
Chemical formula						
Molecular weight [g mol <sup>-1</sup> ]	248.07					
Crystal system	Monoclinic	Triclinic	Monoclinic	Monoclinic	Triclinic	Triclinic
Space group	$P2_1/n$	$P-1$	$P2_1/c$	$P2_1/c$	$P-1$	$P-1$
$a$ [Å]	4.8071(5)	9.1199(2)	6.13189(7)	6.50385(6)	7.62288(4)	6.3963(6)
$b$ [Å]	11.8376(12)	9.3988(2)	8.33230(7)	9.14767(10)	10.1896(4)	6.9500(8)
$c$ [Å]	7.6113(8)	12.1476(9)	25.5961(2)	23.3299(3)	10.2679(5)	7.4999(5)
$\alpha$ [°]	90	88.347(6)	90	90	111.223(4)	76.297(8)
$\beta$ [°]	91.639(9)	75.595(5)	92.4823(9)	92.2350(10)	102.736(4)	80.488(7)
$\gamma$ [°]	90	61.572(4)	90	90	102.750(4)	84.745(8)
$V$ [Å <sup>3</sup> ]	4.32.94	881.981	1306.55	1386.96	684.949	318.98
$Z$	2	2	2	2	1	1
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.90	1.46	1.43	1.50	1.52	1.70
$T$ [K]	85	85	85	85	85	85
	Recryst. from hot water by layering CH <sub>3</sub> CN antisolvent containing pH adjusting additives	Slow evaporation			Solid components heated to 120 °C, subsequently slowly cooled to RT	

Further characterization of the BTATz co-crystals with DMF, pyridine, pyridine-*N*-oxide, 2-pyridone and pyrazine can be found in Kent et al.<sup>[10]</sup>

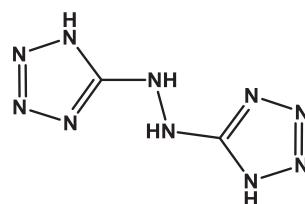
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- [12] S.-T. Yue, S.-Q. Yang, *Chinese J. Energet. Mater.*, **2004**, *28*, 155–157.

## 5,5'-Bis(1*H*-tetrazolyl)hydrazine

Name [German, acronym]: 5,5'-Bistetrazolyl-hydrazine, *N,N'*-bis-(1*H*-tetrazol-5-yl)-hydrazine, 1,2-ditetrazolylhydrazine, 5,5'-hydrazinebistetrazole, bis(5-tetrazole)-hydrazine, 5,5'-Hydrazo-bistetrazole, [5,5'-bis(1*H*-tetrazolyl)hydrazin, *N,N'*-bis[tetrazolyl-(5)]-hydrazin, bis-tetrazolinyliden-hydrazin, BTB, HBT]

Main (potential) use: Possible new high-performance, environmentally friendly energetic material with low sensitivity for use in solid propellants or in propellant charges<sup>[2]</sup>

Structural formula:



	<b>BTB</b>
Formula	C <sub>2</sub> H <sub>4</sub> N <sub>10</sub>
Molecular mass [g mol <sup>-1</sup> ]	168.12
Appearance at RT	White powder <sup>[2]</sup> , white amorphous powder <sup>[4]</sup>
IS [J]	>30 (BAM) <sup>[2]</sup>
FS [N]	>108 (BAM) <sup>[2]</sup>
ESD [J]	No sensitivity toward electric discharge of ~20 kV (Tesla coil) <sup>[2]</sup>
<i>N</i> [%]	83.31
Ω(CO <sub>2</sub> ) [%]	-57.1
T <sub>m.p.</sub> [°C]	dec. @ 208 °C <sup>[2]</sup> , 206.9 – 208.2 (dec., Büchi) <sup>[2]</sup>
T <sub>dec.</sub> [°C]	208 (DSC @ 5 °C/min) <sup>[2]</sup> , 206.9–208.2 (dec., Büchi) <sup>[2]</sup> , 208 <sup>[3]</sup> , 240–241 <sup>[4]</sup>
ρ [g cm <sup>-3</sup> ]	1.841 (X-ray) <sup>[2]</sup> , 1.84 <sup>[3]</sup>
Heat of formation	2,566 cal/g ( $\Delta_f U^\circ$ , calcd.) <sup>[2]</sup> , 2,463 cal/g ( $\Delta_f H^\circ$ , calcd.) <sup>[2]</sup> , 135 kcal/mol ( $Q_f$ @ 25 °) <sup>[4]</sup>
Heat of combustion	-2,396 cal/g ( $\Delta_c U^\circ$ , calcd.) <sup>[2]</sup> , 459.9 kcal/mol ( $Q_c$ ) <sup>[4]</sup>

	Calcd. (EXPLO5)	Lit. values	Exptl.										
$-\Delta_{\text{ex}}U^\circ [\text{kJ kg}^{-1}]$													
$T_{\text{ex}} [\text{K}]$	2,539 <sup>[2,3]</sup>												
$p_{\text{CJ}} [\text{kbar}]$	27.7 GPa <sup>[2,3]</sup>												
$\text{VoD} [\text{m s}^{-1}]$	8,523 (@ 1.841 g cm <sup>-3</sup> ) <sup>[2,3]</sup>												
$V_0 [\text{L kg}^{-1}]$	782 <sup>[2]</sup> , 783 <sup>[3]</sup>												
Critical diameter [cm]	>8 mm (Koenen steel sleeve test, 15 g sample, class G) <sup>[2]</sup>												
Thermal stability	Stable over measurement: ~300 mg sample, atmospheric pressure @ ~40 °C lower than dec. temperature, 48 h – translates to storage periods of >50 years @ RT (Radex) <sup>[2]</sup>												
Solubility [g/mL]	Difficulty soluble in boiling water <sup>[4]</sup> , insoluble in organic solvents <sup>[4]</sup>												
Compatibility	Some dec. after heating with copper for 6 h @ 170 °C (Radex) <sup>[2]</sup>												
Flame test	Response to thermal shock (s = smokeless, n.s. = non-smokeless combustion) <sup>[2]</sup> :	<table border="1"> <thead> <tr> <th>Sample</th> <th>Neat (powder)</th> <th>Neat (pellet)</th> <th>HBT/AN (1:3)</th> <th>HBT/AND (1:2)</th> </tr> </thead> <tbody> <tr> <td>HBT</td> <td>Deflagrates (s)</td> <td>Deflagrates (s)</td> <td>s</td> <td>s</td> </tr> </tbody> </table>		Sample	Neat (powder)	Neat (pellet)	HBT/AN (1:3)	HBT/AND (1:2)	HBT	Deflagrates (s)	Deflagrates (s)	s	s
Sample	Neat (powder)	Neat (pellet)	HBT/AN (1:3)	HBT/AND (1:2)									
HBT	Deflagrates (s)	Deflagrates (s)	s	s									
	Neat HBT gives bright yellow flame without smoke <sup>[2]</sup>												

Crystals obtained by dissolving small amount of solid in boiling water and allowing to cool.

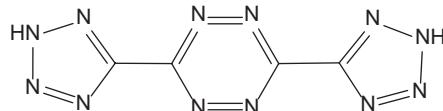
- [1] T. M. Klapötke, D. G. Piercy, F. Rohrbacher, J. Stierstorfer, ZAAC, **2012**, *638*, 2235–2242.
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## 3,6-Bis(tetrazol-5-yl)-1,2,4,5-tetrazine

Name [German, acronym]: 3,6-Bis(tetrazol-5-yl)-1,2,4,5-tetrazine, [3,6-bis(tetrazol-5-yl)-1,2,4,5-tetrazin]

Main (potential) use: secondary explosive, gas generant

Structural formula:



	3,6-Bis(tetrazol-5-yl)-1,2,4,5-tetrazine		
Formula	$C_4H_2N_{12}$		
Molecular mass [g mol <sup>-1</sup> ]	218.14		
Appearance at RT	Red solid <sup>[1]</sup>		
IS [J]	6 (BAM) <sup>[1]</sup>		
FS [N]	72 ( <sup>1</sup> / <sub>6</sub> , BAM) <sup>[1]</sup>		
ESD [J]	0.2 (OZM apparatus) <sup>[1]</sup>		
N [%]	77.05		
$\Omega(CO_2)$ [%]	-66.0		
$T_{dec.}$ [°C]	226 (DSC @ 5 °C/min) <sup>[1]</sup>		
$\rho$ [g cm <sup>-3</sup> ]	1.75 (est.) <sup>[1]</sup>		
Heat of formation	4975.5 kJ/kg ( $\Delta_f U$ ) <sup>[1]</sup>		
	Calcd. (EXPLO5 5.05)	Lit. values	Exptl.
$-\Delta_{ex}U^o$ [kJ kg <sup>-1</sup> ]	5,077 <sup>[1]</sup>		
$T_{ex}$ [K]	3,900 <sup>[1]</sup>		
$p_{C,J}$ [kbar]	281 <sup>[1]</sup>		
VoD [m s <sup>-1</sup> ]	8,295 (@ 1.75 g cm <sup>-3</sup> ) <sup>[1]</sup>		
$V_0$ [L kg <sup>-1</sup> ]	853 <sup>[1]</sup>		
$I_s$ [s]	2,383 (using isobaric (60 bar) conditions) <sup>[1]</sup>		
Solubility [g/mL]	Soluble in DMSO <sup>[1]</sup>		

	<b>C<sub>4</sub>H<sub>6</sub>N<sub>12</sub>O<sub>2</sub><sup>[1]</sup> (dihydrate)</b>
Chemical formula	C <sub>4</sub> H <sub>6</sub> N <sub>12</sub> O <sub>2</sub>
Molecular weight [g mol <sup>-1</sup> ]	254.17
Crystal system	Monoclinic
Space group	P2 <sub>1</sub> /n
<i>a</i> [Å]	10.49718(15)
<i>b</i> [Å]	4.8574(5)
<i>c</i> [Å]	10.5978(14)
α [°]	90
β [°]	113.664(16)
γ [°]	90
<i>V</i> [Å <sup>3</sup> ]	494.93
<i>Z</i>	2
<i>ρ</i> <sub>calc</sub> [g cm <sup>-3</sup> ]	1.706
<i>T</i> [K]	173

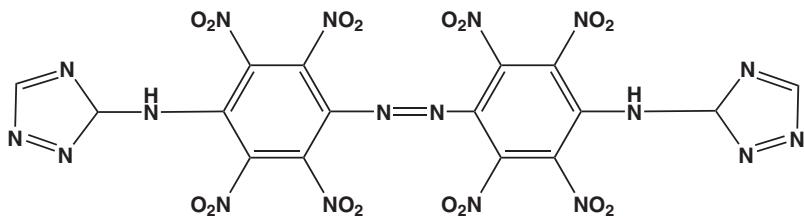
[1] T. M. Klapötke, D. G. Piercy, F. Rohrbacher, J. Stierstorfer, ZAAC, **2012**, 638, 2235–2242.

**N,N'-Bis(1,2,4-triazol-3-yl)-4,4'-diamino-2,2',3,3',5,5',6,6'-octanitroazobenzene**

Name [German, acronym]: N,N'-Bis(1,2,4-triazol-3-yl)-4,4'-diamino-2,2',3,3',5,5',6,6'-octanitroazobenzene [N,N'-bis(1,2,4-triazol-3-yl)-4,4'-diamino-2,2',3,3',5,5',6,6'-octanitroazobenzol, BTDAONAB]

Main (potential) use: Patented for use as explosive component in downhole uses<sup>[4]</sup>, most thermally stable explosive reported so far, reported on laboratory scale and needs further investigation<sup>[6]</sup>

Structural formula:



	<b>BTDAONAB</b>		
Formula	$C_{16}H_8N_{18}O_{16}$		
Molecular mass [g mol <sup>-1</sup> ]	708.35		
Appearance at RT			
IS [J]	87 cm <sup>[1,2,3,6]</sup>		
N [%]			
$\Omega(CO_2)$ [%]	-45.2		
$T_{m.p.}$ [°C]	>350 <sup>[2]</sup> , does not melt/show any change before exotherm @ 550 °C <sup>[6]</sup>		
$T_{\text{phase transition}}$ [°C]	Does not melt/show any change before exotherm @ 550 °C <sup>[6]</sup>		
$T_{\text{dec.}}$ [°C]	>550 <sup>[1,3]</sup> , 550 (exo, DTA) <sup>[1,2,3]</sup> , 550 (exo, DSC) <sup>[4]</sup>		
$\rho$ [g cm <sup>-3</sup> ]	1.97 <sup>[1,2,3,5,6]</sup> , 1.948 (calcd., EDPHT 2.0) <sup>[5]</sup> , 1.825 (calcd., Ammon) <sup>[5]</sup>		
Heat of formation			
	Calcd. (EXPL05 6.03)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^{\circ}$ [kJ kg <sup>-1</sup> ]			

$T_{\text{ex}}$ [K]			
$p_{\text{CJ}}$ [kbar]			
VoD [ $\text{m s}^{-1}$ ]		8,321 ( $\rho$ not specified) <sup>[4]</sup>	
$V_0$ [ $\text{L kg}^{-1}$ ]			

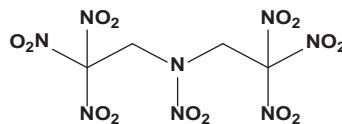
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- [2] J. P. Agrawal, *Propellants, Explosives, Pyrotechnics*, 2005, 30, 316–328.
- [3] J. P. Agrawal, Mehilal, A. K. Sikder, N. Sikder, *Ind. J. Eng. Mater. Sci.*, 2004, 11, 516–520.
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## Bis(trinitroethyl)nitramine

Name [German, acronym]: Bi-trinitroethylnitramine, *N,N*-bis(2,2,2-trinitroethyl)nitramide, bis(2,2,2-trinitroethyl)-nitramine [di(2,2,2-trinitroethyl)nitramin, BTNENA, BTNEN, HOX, BTNNA]

Main (potential) use: Oxidizer

Structural formula:



	HOX		
Formula	$\text{C}_4\text{H}_4\text{N}_8\text{O}_{14}$		
Molecular mass [g mol <sup>-1</sup> ]	388.12		
Appearance at RT			
IS [J]	5 cm with 2.5 kg hammer <sup>[6]</sup> , $H_{50} = 5 \text{ cm}$ <sup>[8,19]</sup> , $H_{50\%} = 12\text{--}15 \text{ cm}$ (2 kg mass) <sup>[10]</sup> , 2.5 (BAM) <sup>[11]</sup> , $H_{50} = 5 \text{ cm}$ (2.5 kg mass, type 12 tool) <sup>[26]</sup> , $A_{d1} = 92\%$ , $A_{d2} = 74\%$ , $LL = 0.6 \text{ m}$ , $A_{50\ d1} = 0.9 \text{ m}$ , $A_{50\ d2} = 1.7$ <sup>[12]</sup> , $H_{50\%} = 10 \text{ cm}$ (2.5 kg mass) <sup>[28]</sup>		
FS [N]	12 kp (Julius-Peters apparatus) <sup>[11]</sup> , $p_{\text{fr},\text{LL}} = 100 \text{ MPa}$ <sup>[12]</sup> , $p_{\text{fr},50\%} = 250 \text{ MPa}$ <sup>[12]</sup>		
$N$ [%]	28.87		
$\Omega(\text{CO}_2)$ [%]	+16.5		
$T_{\text{m.p.}}$ [°C]	95 <sup>[11,14]</sup> , 94–96 <sup>[10]</sup> , dec. <sup>[20]</sup> , 94 <sup>[28]</sup>		
$T_{\text{dec.}}$ [°C]	Rapid dec. above mpt. <sup>[10]</sup> , 171 <sup>[11]</sup> , 94.5 <sup>[20]</sup>		
$\rho$ [g cm <sup>-3</sup> ]	$2.028 \pm 0.06$ (@ 293.15 K) <sup>[1]</sup> , 1.91 (@ 20 °C) <sup>[10]</sup> , 1.92 (crystal) <sup>[11]</sup> , 1.953 <sup>[19]</sup> , 1.97 (measured, mean density) <sup>[20]</sup> , 1.96 (crystal) <sup>[28]</sup>		
Heat of formation	$-27.6 \text{ kJ/mol}$ ( $\Delta H_f^\circ$ ) <sup>[2]</sup> , $-71.2 \text{ kJ kg}^{-1}$ ( $\Delta H_f^\circ$ ) <sup>[2]</sup> , $-63 \text{ kJ/kg}$ ( $\Delta H_f^\circ$ ) <sup>[4]</sup> , $-6.69 \text{ kcal/mol}$ ( $\Delta H_f^\circ$ (s)) <sup>[19]</sup> , $-17.0 \text{ kcal/kg}$ (enthalpy of form.) <sup>[21]</sup> , 12 kcal/mol (calcd.) <sup>[28]</sup> , $-28.0 \text{ kJ/mol}$ (enthalpy of form., exptl.) <sup>[29]</sup> , $-23.1 \text{ kJ/mol}$ (enthalpy of form., calcd., emp.) <sup>[29]</sup> , $-39.8 \text{ kJ/mol}$ (enthalpy of form., calcd., S-D method) <sup>[29]</sup> , $-27.9 \pm 2.0 \text{ kJ/mol}$ ( $\Delta H_f^\circ$ , (c)) <sup>[30]</sup> , $89.6 \pm 2.2 \text{ kJ/mol}$ ( $\Delta H_f^\circ$ , (g)) <sup>[30]</sup>		
Heat of combustion	$Q_c = 1,355 \text{ cal/g}$ <sup>[10]</sup>		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.

$-\Delta_{\text{ex}}U^0 [\text{kJ kg}^{-1}]$	3,287	1,297 cal/g <sup>[18]</sup> 1.25 kcal/g ( $Q_{\text{max.}}$ , calcd.) <sup>[19]</sup> 1,250 kcal/kg (@ 1.600 g cm <sup>-3</sup> , calcd.) [H <sub>2</sub> O vapor] <sup>[21]</sup>	5,436 [H <sub>2</sub> O (l)] <sup>[2]</sup> 5,397 <sup>[4]</sup> 1,250 [H <sub>2</sub> O (g)] <sup>[7]</sup> 4,857 <sup>[9]</sup> 1,250 kcal/kg (@ 1.600 g cm <sup>-3</sup> ) [H <sub>2</sub> O vapor] <sup>[21]</sup>
$T_{\text{ex}} [\text{K}]$	2,518		
$p_{\text{CJ}} [\text{kbar}]$	325	345 (@ 1.927 g cm <sup>-3</sup> , calcd., empirical, Xiang) <sup>[18]</sup>  369 (@ 1.953 g cm <sup>-3</sup> , calcd.) <sup>[19]</sup>	31.9 GPa <sup>[16]</sup>  357.6 (@ 1.927 g cm <sup>-3</sup> ) <sup>[18]</sup>
VoD [m s <sup>-1</sup> ]	8,913 (@ TMD)	8,690 (@ 1.96 g cm <sup>-3</sup> (TMD), calcd. R-P-method) <sup>[17]</sup>  8,710 (@ 1.96 g cm <sup>-3</sup> (TMD), Aizenshtadt method) <sup>[17]</sup>  9,050 (@ 1.96 g cm <sup>-3</sup> (TMD), K-J) <sup>[17]</sup>  8,910 (@ 1.953 g cm <sup>-3</sup> , calcd.) <sup>[19]</sup>	7,180 (@ 1.5 g cm <sup>-3</sup> ) <sup>[10]</sup>  8,520 (@ 1.9 g cm <sup>-3</sup> ) <sup>[10]</sup>  8,850 (@ 1.96 g cm <sup>-3</sup> ) <sup>[3]</sup>  8,750 (@ 1.960 g cm <sup>-3</sup> ) <sup>[4]</sup>  8,610 (@ 1.88 g cm <sup>-3</sup> ) <sup>[16]</sup>  8,700 (@ 1.93 g cm <sup>-3</sup> ) <sup>[16]</sup>  8,570 (@ 1.82 g cm <sup>-3</sup> ) <sup>[16]</sup>  8,657 (@ 1.925 g cm <sup>-3</sup> ) <sup>[18]</sup>
$V_0 [\text{L kg}^{-1}]$	721		693 <sup>[2,5]</sup>  705 <sup>[9]</sup>

Critical pressure of explosion initiation [GPa]	$p_{cr} = 0.40 \pm 0.01^{[23,24]}$ , ( $\sigma_{ult} = 50 \text{ MPa}^{[23,24]}$ ), $p_{ult} = 0.79 \pm 0.02^{[23,24]}$ , $p_{cr} = 0.79 \pm 0.02^{[25]}$ , critical initiation pressure = $0.79 \pm 0.02 \text{ GPa}^{[27]}$																																																								
Trauzl test [cm <sup>3</sup> , % TNT]	147–148% TNT <sup>[13]</sup>																																																								
Ballistic mortar test	134–135% TNT <sup>[13]</sup>																																																								
5 s explosion $T$ [°C] 5 s ignition $T$ [°C]	200 <sup>[10]</sup>																																																								
Solubility [g/mL]	Approx. solubility limit in nitropolymers (weight percent) <sup>[28]</sup> : 70 in NC (12.6% N) <sup>[28]</sup> , 75 in NC (13.45% N) <sup>[28]</sup> , 65 in polynitropolyurethane <sup>[28]</sup> , 75 in polydinitropropylacrylate <sup>[28]</sup>																																																								
Cylinder velocities	$\rho = 1.80 \text{ g cm}^{-3}$ , Cu cylinder, $R$ = current value of outer radius of cylinder, $R_0$ = initial value of outer radius of cylinder <sup>[22]</sup> : <table border="1" style="margin-left: 20px;"> <thead> <tr> <th><math>\rho = 1.90 \text{ g cm}^{-3}</math></th> <th colspan="6"><math>R - R_0</math> (mm)</th> </tr> </thead> <tbody> <tr> <td>Exptl.</td> <td>1.52</td> <td>1.57</td> <td>1.65</td> <td>1.72</td> <td>1.75</td> <td>1.78</td> </tr> <tr> <td>1</td> <td>1.49</td> <td>1.55</td> <td>1.62</td> <td>1.69</td> <td>1.72</td> <td>1.75</td> </tr> <tr> <td>2</td> <td>1.48</td> <td>1.54</td> <td>1.61</td> <td>1.68</td> <td>1.71</td> <td>1.74</td> </tr> </tbody> </table> <table border="1" style="margin-left: 20px;"> <thead> <tr> <th><math>\rho = 1.85 \text{ g cm}^{-3}</math></th> <th colspan="6"><math>R - R_0</math> (mm)</th> </tr> </thead> <tbody> <tr> <td>Exptl.</td> <td>1.48</td> <td>1.53</td> <td>1.61</td> <td>1.68</td> <td>1.71</td> <td>1.74</td> </tr> <tr> <td>1</td> <td>1.46</td> <td>1.52</td> <td>1.59</td> <td>1.65</td> <td>1.68</td> <td>1.72</td> </tr> <tr> <td>2</td> <td>1.45</td> <td>1.51</td> <td>1.58</td> <td>1.64</td> <td>1.67</td> <td>1.71</td> </tr> </tbody> </table>	$\rho = 1.90 \text{ g cm}^{-3}$	$R - R_0$ (mm)						Exptl.	1.52	1.57	1.65	1.72	1.75	1.78	1	1.49	1.55	1.62	1.69	1.72	1.75	2	1.48	1.54	1.61	1.68	1.71	1.74	$\rho = 1.85 \text{ g cm}^{-3}$	$R - R_0$ (mm)						Exptl.	1.48	1.53	1.61	1.68	1.71	1.74	1	1.46	1.52	1.59	1.65	1.68	1.72	2	1.45	1.51	1.58	1.64	1.67	1.71
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	BTNEN/HOX <sup>[14]</sup>	BTNEN/HOX <sup>[15]</sup>	BTNEN/HOX <sup>[14]</sup>
Chemical formula	C <sub>4</sub> H <sub>4</sub> N <sub>8</sub> O <sub>14</sub>	C <sub>4</sub> H <sub>4</sub> N <sub>8</sub> O <sub>14</sub>	C <sub>4</sub> H <sub>4</sub> N <sub>8</sub> O <sub>14</sub>
Molecular weight [g mol <sup>-1</sup> ]	388.12	388.12	388.12
Crystal system	Orthorhombic	Monoclinic	Monoclinic
Space group	Pn21a	P2 <sub>1</sub> /n (no. 14)	P2 <sub>1</sub> /a (no. 14)
<i>a</i> [Å]	22.995(20)	11.820	20.654(10)
<i>b</i> [Å]	9.506(8)	6.162	11.809(7)
<i>c</i> [Å]	6.147(4)	18.229	6.162(2)
$\alpha$ [°]	90	90	90
$\beta$ [°]	90	96.1	90
$\gamma$ [°]	90	90	118.65(3)

$V [\text{\AA}^3]$	1,343.68	1,320.19	1,318.92
$Z$	4	4	4
$\rho_{\text{calc}} [\text{g cm}^{-3}]$	1.91858	1.953	1.95459
$T [\text{K}]$	295	295	295

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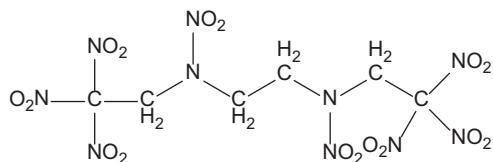
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## Bis(2,2,2-trinitroethyl-*N*-nitro) ethylenediamine

Name [German, acronym]: *N,N'*-(Ethane-1,2-diyl)bis(*N*-(2,2,2-trinitroethyl)nitramide), *N,N'*-bis[N-(2,2,2-trinitroethyl)-*N*-nitro]ethylenediamine [ZOX, BTNEDA]

Main (potential) use: Can be used in EBW detonators, explosive trains and other special applications; in production in China since 1969<sup>[1]</sup>, high explosive<sup>[5]</sup>

Structural formula:



	<b>ZOX</b>
Formula	C <sub>6</sub> H <sub>8</sub> N <sub>10</sub> O <sub>16</sub>
Molecular mass [g mol <sup>-1</sup> ]	476.18
Appearance at RT	
IS [J]	10 kg hammer weight, drop height = 25 cm, % explosions: 100% ZOX, cf. 80% RDX, 100% HMX, 100% PETN <sup>[1]</sup> , $H_{50\%} = 15.03$ cm (predicted, cf. 15.60 cm for PETN) <sup>[5]</sup> $A_{d1} = >100\%$ (calcd.), 100% (exptl.), $A_{d2} = 76\%$ (calcd.), 100% (exptl.), $LL = 0.4$ m (calcd.), 0.3 m (exptl.), $A_{50\%d1} = 1.1$ m (calcd.), 0.5 m (exptl.), $A_{50\%d2} = 1.0$ m (calcd.), 0.5 m (exptl.) <sup>[3]</sup>
FS [N]	Kazlov friction test, pendular angle = 90 °, gauge pressure = 25 kg/cm <sup>2</sup> , % explosions: 88% ZOX cf. 4% RDX, 28% HMX, 32% PETN <sup>[1]</sup> Kazlov friction test, pendular angle = 90 °, gauge pressure = 40 kg/cm <sup>2</sup> , % explosions: 100% ZOX cf. 76% RDX, 100% HMX, 92% PETN <sup>[1]</sup> $p_{fr., LL} = 150$ MPa (calcd.), 100 MPa (exptl.), $p_{fr., 50\%} = 310$ MPa (calcd.), 250 (exptl.) <sup>[3]</sup>
N [%]	29.42
$\Omega(\text{CO}_2)$ [%]	0
$T_{\text{m.p.}}$ [°C]	179.2–181.5 <sup>[1]</sup> , 180 (endo, DSC @ 10 °C/min) <sup>[5,6]</sup>
$T_{\text{phase transition}}$ [°C]	No phase change observed in DSC @ 10 °C/min <sup>[5]</sup>

$T_{\text{dec.}} [\text{°C}]$	197 (exo, DSC @ 10 °C/min) <sup>[5,6]</sup>		
Nonisothermal DSC <sup>[5]</sup> :			
Heating rate, $\beta (\text{K min}^{-1})$	$T_e (\text{K})$ (onset)	$T_p (\text{K})$ (max. peak $T$ )	
1.053	445.15	450.15	
2.105	453.15	457.15	
5.294	460.15	463.15	
10.56	467.15	470.15	
20.63	472.15	476.15	
DSC sample purity = >99.5% <sup>[6]</sup> :			
Heating rate, $\beta (\text{K min}^{-1})$		$T_p (\text{°C})$ (max. peak $T$ )	
1.053		177	
2.105		184	
5.294		190	
10.56		197	
20.63		203	
$\rho [\text{g cm}^{-3}]$	1.87 (crystal) <sup>[1,2,5,6]</sup>		
Heat of formation	53.5 kJ/mol <sup>[1]</sup> , 14 kJ/kg ( $\Delta H_f^\circ$ ) <sup>[4]</sup> , $-53.54 \pm 6.41$ kJ/mol ( $\Delta H_f^\circ_m$ (s, 298.15 K)) <sup>[5]</sup>		
Heat of combustion	$7.25 \text{ MJ/kg}^{[1]}$ , $\Delta_c U_{(\text{s}, 298.15 \text{ K})} = -3478.11 \pm 6.41 \text{ kJ/mol}$ (constant volume, standard combustion energy) <sup>[5]</sup>		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{\text{ex}} U^\circ [\text{kJ kg}^{-1}]$		1,704 kcal/kg (calcd.) <sup>[1]</sup> $Q_{\text{cal}} = 6426 \text{ kJ/kg}^{[4]}$ 6,879.7 J/g (@ 1.87 $\text{g cm}^{-3}$ , $\Delta H_f^\circ = -53.54$ kJ/mol, calcd., K-J) <sup>[5]</sup>	1,542 kcal/kg <sup>[1]</sup>
$T_{\text{ex}} [\text{K}]$			

$p_{CJ}$ [kbar]		35.0 GPa (@ 1.875 g cm <sup>-3</sup> ) <sup>[4]</sup>  39.23 GPa (@ 1.87 g cm <sup>-3</sup> , $\Delta H_f^\circ = -53.54$ kJ/mol, calcd., K-J) <sup>[5]</sup>	37.8 ± 0.3 GPa (@ 1.840 g cm <sup>-3</sup> , PB-ZOX-9159* (95% ZOX)) <sup>[1]</sup>																																												
VoD [m s <sup>-1</sup> ]		9,100 (@ 1.875 g cm <sup>-3</sup> ) <sup>[4]</sup>  ~8,970 (@ 1.842 g cm <sup>-3</sup> )  9,298 (@ 1.87 g cm <sup>-3</sup> , $\Delta H_f^\circ = -53.54$ kJ/mol, calcd., K-J) <sup>[5]</sup>	8,970 (@ 1.842 g cm <sup>-3</sup> , 10 mm charge diameter) <sup>[1]</sup>  8,816 ± 6 (@ 1.840 g cm <sup>-3</sup> , PB-ZOX- 9,159* (95% ZOX)) <sup>[1]</sup>																																												
$V_0$ [L kg <sup>-1</sup> ]		0.0315 mol·g <sup>-1</sup> (@ 1.87 g cm <sup>-3</sup> , $\Delta H_f^\circ = -53.54$ kJ/mol, calcd., K-J, $M_g = 31.73$ g mol <sup>-1</sup> ) <sup>[5]</sup>	0.712 m <sup>3</sup> /kg (specific volume of detonation products) <sup>[1]</sup>																																												
Critical diameter [cm]	0.2 mm (ZOX/silicon resin, 80/20, open channels of Al plate) <sup>[1]</sup>																																														
Critical initial density [g cm <sup>-3</sup> ]	1.71 <sup>[2]</sup>																																														
$p_{cr}$ [GPa]	1.5 (calcd.) <sup>[4]</sup>																																														
Critical $T$ for thermal explosion, $T_b$ [K]	449.88 <sup>[5]</sup> , 455.28 <sup>[5]</sup> , 446.69 <sup>[5]</sup> , 452.92 <sup>[5]</sup> , 449.76 <sup>[5]</sup> , 455.14 <sup>[5]</sup> , 439.81 <sup>[5]</sup> , 435.75 <sup>[5]</sup> , 182.2 <sup>[6]</sup>																																														
5 s explosion $T$ [°C]	232 <sup>[1]</sup>																																														
Thermal stability	<p>Bourdon glass barometer, time needed for 0.01% decomposition<sup>[1]</sup>:</p> <table border="1"> <thead> <tr> <th><math>T</math> (°C)</th> <th>70</th> <th>85</th> <th>100</th> <th>115</th> <th>130</th> </tr> </thead> <tbody> <tr> <td><math>t_{0.01\%}</math> (min)</td> <td>65,760</td> <td>7,428</td> <td>1,212</td> <td>567</td> <td>28.2</td> </tr> </tbody> </table> <p>Initial decomposition velocity, <math>W_0</math> (mL/min.g) and half-life, <math>t_{0.5}</math> (min)<sup>[1]</sup>:</p> <table border="1"> <thead> <tr> <th rowspan="2"><math>T</math> (°C)</th> <th colspan="2">130</th> <th colspan="2">150</th> <th colspan="2">160</th> <th colspan="2">170</th> </tr> <tr> <th><math>W_0</math></th> <th><math>t_{0.5}</math></th> <th><math>W_0</math></th> <th><math>t_{0.5}</math></th> <th><math>W_0</math></th> <th><math>t_{0.5}</math></th> <th><math>W_0</math></th> <th><math>t_{0.5}</math></th> </tr> </thead> <tbody> <tr> <td>ZOX</td> <td>0.001</td> <td>9,540</td> <td>0.032</td> <td>449.5</td> <td>0.090</td> <td>110.3</td> <td>0.30</td> <td>26.0</td> </tr> </tbody> </table> <p>Industrial-grade ZOX<sup>[1]</sup>:</p> <table border="1"> <thead> <tr> <th>BGET, 120 °C, 48 h, mL/1 g</th> <th>CRT, 150 °C, 2 h, mL/1 g</th> <th>TG, 100 °C, 48 h, %</th> </tr> </thead> <tbody> <tr> <td>1.861</td> <td>3.9</td> <td>0.06</td> </tr> </tbody> </table>			$T$ (°C)	70	85	100	115	130	$t_{0.01\%}$ (min)	65,760	7,428	1,212	567	28.2	$T$ (°C)	130		150		160		170		$W_0$	$t_{0.5}$	$W_0$	$t_{0.5}$	$W_0$	$t_{0.5}$	$W_0$	$t_{0.5}$	ZOX	0.001	9,540	0.032	449.5	0.090	110.3	0.30	26.0	BGET, 120 °C, 48 h, mL/1 g	CRT, 150 °C, 2 h, mL/1 g	TG, 100 °C, 48 h, %	1.861	3.9	0.06
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Vacuum stability test [cm <sup>3</sup> /h]	VST 120 °C, 48 h, mL/5 g = 3.7 (ZOX, industrial grade) <sup>[1]</sup>  Effect of recryst. process on thermal stability of ZOX <sup>[1]</sup> :  <table border="1"> <thead> <tr> <th>Process of recryst.</th><th>VST 100 °C, 48 h, mL/g</th></tr> </thead> <tbody> <tr> <td>ZOX recryst. from ethyl acetate-benzene</td><td>0.09, 0.24</td></tr> <tr> <td>ZOX precipitated by pouring acetone soln. to cool water with Agitation</td><td>8.7</td></tr> </tbody> </table>	Process of recryst.	VST 100 °C, 48 h, mL/g	ZOX recryst. from ethyl acetate-benzene	0.09, 0.24	ZOX precipitated by pouring acetone soln. to cool water with Agitation	8.7																		
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Solubility [g/mL]	Soluble in acetone, dioxane, methyl acetate, ethyl acetate <sup>[1]</sup> , slightly soluble in MeOH, EtOH and acetic anhydride <sup>[1]</sup> , insoluble in water, Et <sub>2</sub> O, benzene, toluene, CHCl <sub>3</sub> , CCl <sub>4</sub> and dichloroethane <sup>[1]</sup>  Approx. solubilities in g (ZOX)/100 g solvent @ various T (°C) <sup>[1]</sup> : solvent = acetone, 25 g @ 20 °C, 31 g @ 30 °C, 38 g @ 40 °C, 45 g @ 50 °C, 52 g @ 60 °C <sup>[1]</sup> solvent = methyl acetate, 8 g @ 20 °C, 9 g @ 30 °C, 12 g @ 40 °C, 15 g @ 50 °C, 20 g @ 60 °C <sup>[1]</sup> solvent = nitromethane, 2 g @ 20 °C, 3 g @ 30 °C, 4 g @ 40 °C, 5 g @ 50 °C, 8 g @ 60 °C, 17 g @ 80 °C, 32 g @ 90 °C, 43 g @ 100 °C <sup>[1]</sup> solvent = dioxane, 1 g @ 20 °C, 2 g @ 30 °C, 3 g @ 40 °C, 4 g @ 50 °C, 6 g @ 60 °C, 10 g @ 70 °C, 15 g @ 80 °C, 20 g @ 90 °C <sup>[1]</sup>																								
Compatibility	Relatively stable in acids, but sensitive to alkalis <sup>[1]</sup> , compatibility of ZOX with related materials is poor, only few binders and phlegmatizers such as silicon rubber, fluororubber and fluorographite are compatible with ZOX <sup>[1]</sup>  Compatibility data of ZOX in VST (120 °C, 48 h) <sup>[1]</sup> :  <table border="1"> <thead> <tr> <th>Material</th> <th>mL/5 g</th> <th>Mixture (1:1)</th> <th>mL/5 g</th> </tr> </thead> <tbody> <tr> <td>ZOX</td> <td>3.70</td> <td>ZOX/nylon</td> <td>Explodes</td> </tr> <tr> <td>F<sub>2314</sub></td> <td>1.15</td> <td>ZOX/F<sub>2314</sub></td> <td>4.15</td> </tr> <tr> <td>Polyisobutylene</td> <td>0.25</td> <td>ZOX/PIB</td> <td>96.35</td> </tr> <tr> <td>Silicon resin</td> <td>2.65</td> <td>ZOX/silicon resin</td> <td>2.60</td> </tr> <tr> <td>Wax</td> <td>0.55</td> <td>ZOX/wax</td> <td>87.45</td> </tr> </tbody> </table>	Material	mL/5 g	Mixture (1:1)	mL/5 g	ZOX	3.70	ZOX/nylon	Explodes	F <sub>2314</sub>	1.15	ZOX/F <sub>2314</sub>	4.15	Polyisobutylene	0.25	ZOX/PIB	96.35	Silicon resin	2.65	ZOX/silicon resin	2.60	Wax	0.55	ZOX/wax	87.45
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Plate push test	$\rho = 1.840 \text{ g cm}^{-3}$ , $U_f = 4632 \pm 22 \text{ m/s}$ , $1/2U_f^2 = 10.73 \text{ kJ/g}$ (PB-ZOX-9159*) <sup>[1]</sup>																								
Cylinder test	$\rho = 1.802 \text{ g cm}^{-3}$ (97.1% TMD), $E(19 \text{ mm}) = 1.722 \text{ kJ/g}$ (PB-ZOX-9159*) <sup>[1]</sup>																								
Thermal conductivity, $\lambda$	0.269 W·(m·K <sup>-1</sup> ) <sup>[5]</sup>																								
Bridgewire	ZOX is more easily initiated by shock wave and bridgewire than PETN <sup>[1]</sup>																								

\* PB-ZOX-9159 is a mixture of ZOX with the same additives as those of PB-HMX-9159.

	<b>ZOX<sup>[1]</sup></b>
Chemical formula	C <sub>6</sub> H <sub>8</sub> N <sub>10</sub> O <sub>16</sub>
Molecular weight [g mol <sup>-1</sup> ]	
Crystal system	Monoclinic
Space group	
<i>a</i> [Å]	5.9767
<i>b</i> [Å]	12.0146
<i>c</i> [Å]	11.8436
$\alpha$ [°]	90
$\beta$ [°]	97.171
$\gamma$ [°]	90
<i>V</i> [Å <sup>3</sup> ]	
<i>Z</i>	2
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.88
<i>T</i> [K]	

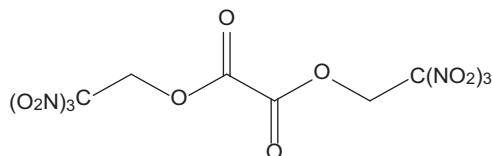
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## 2,2,2-Bis(trinitroethyl) oxalate

Name [German, acronym]: 2,2,2-Bis(trinitroethyl) oxalate [BTOx]

Main (potential) use: Oxidizer

Structural formula:



	BTOx
Formula	C <sub>6</sub> H <sub>4</sub> N <sub>6</sub> O <sub>16</sub>
Molecular mass [g mol <sup>-1</sup> ]	416.1
Appearance at RT	
IS [J]	10 <sup>[1]</sup> , H <sub>50</sub> = 15 cm (2.5 kg mass, type 12 tool) <sup>[2]</sup>
FS [N]	>360 <sup>[1]</sup>
ESD [J]	0.7 <sup>[1]</sup>
N [%]	20.2
Ω(CO <sub>2</sub> ) [%]	+7.7
T <sub>m.p.</sub> [°C]	115
T <sub>dec.</sub> [°C]	186 (DSC @ 5 °C/min) <sup>[1]</sup>
ρ [g cm <sup>-3</sup> ]	1.84 (@ 298 K) <sup>[1]</sup>
Heat of formation	-688 kJ/mol (ΔH <sup>o</sup> <sub>f</sub> ) <sup>[1]</sup> , -1,576 kJ kg <sup>-1</sup> (ΔH <sup>o</sup> <sub>f</sub> ) <sup>[1]</sup>
	Calcd. (EXPLO5 6.03)
	AP as oxidizer
I <sub>sp</sub> [s] (neat) <sup>a</sup>	231
I <sub>sp</sub> [s] (neat) <sup>b</sup>	293
I <sub>sp</sub> [s] <sup>a,c</sup> (71% oxidizer)	250
I <sub>sp</sub> [s] <sup>b,c</sup> (71% oxidizer)	319
330	

<sup>a</sup>70 bar/1 bar, isobaric combustion, equilibrium to throat and frozen to exit.

<sup>b</sup>70 bar, 1 mbar, isobaric combustion, equilibrium to throat and frozen to exit.

<sup>c</sup>15% Al; 6% polybutadiene acrylic acid, 6% polybutadiene acrylonitrile, and 2% bisphenol A ether.

	<b>BTOx<sup>[1]</sup></b>
Chemical formula	C <sub>6</sub> H <sub>4</sub> N <sub>6</sub> O <sub>16</sub>
Molecular weight [g mol <sup>-1</sup> ]	416.12
Crystal system	Monoclinic
Space group	P2 <sub>1</sub> /c (14)
<i>a</i> [Å]	10.5849(5)
<i>b</i> [Å]	21.6214(11)
<i>c</i> [Å]	6.5071(3)
α [°]	90
β [°]	98.485(5)
γ [°]	90
<i>V</i> [Å <sup>3</sup> ]	1,472.92(12)
<i>Z</i>	4
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.877
<i>T</i> [K]	173

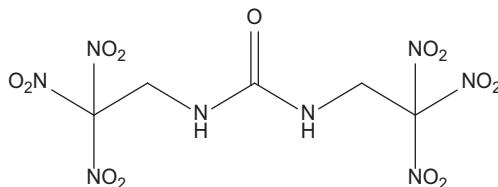
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## Bis(trinitroethyl)urea

Name [German, acronym]: 1,3-Bis(2,2,2-trinitroethyl)urea, bis-trinitroethylurea, *N,N'*-bis( $\beta,\beta,\beta$ -trinitroethylurea), hexanitrodiethyl urea, 1,3-di(2,2,2-trinitroethyl)-urea [di(2,2,2-trinitroethyl)-Harnstoff, BTNEU]

Main (potential) use: Component of pyrotechnics, synthetic intermediate

Structural formula:



	<b>BTNEU</b>		
Formula	C <sub>5</sub> H <sub>6</sub> N <sub>8</sub> O <sub>13</sub>		
Molecular mass [g mol <sup>-1</sup> ]	386.15		
Appearance at RT			
IS [J]	3.92 (2.5 kg mass) <sup>[8]</sup> , 17 cm (2.5 kg hammer) <sup>[10]</sup> , log H <sub>50%</sub> = 1.23 <sup>[12]</sup> , H <sub>50</sub> = 17 cm <sup>[13]</sup> , H <sub>50</sub> = 17 cm (2.5 kg mass, type 12 tool) <sup>[23]</sup>		
FS [N]	ABL 457 lbs <sup>[8]</sup>		
ESD [J]	0.25 J ( <sup>10</sup> / <sub>10</sub> NF) <sup>[8]</sup>		
N [%]	29.02		
$\Omega(\text{CO}_2)$ [%]	±0		
T <sub>m.p.</sub> [°C]	185–186 <sup>[1]</sup> , 187–191 (dec., crystals) <sup>[16]</sup>		
$\rho$ [g cm <sup>-3</sup> ]	1.906 ± 0.06 (@ 293 K) <sup>[2]</sup> , 1.861 <sup>[5]</sup> , 1.85 (measured, flotation method) <sup>[15]</sup>		
Heat of formation	-360.8 kJ/mol ( $\Delta_f H^\circ$ , calcd.) <sup>[3]</sup> , 305.0 kJ/mol ( $\Delta_f H^\circ$ ) <sup>[7]</sup> , -189.0 kcal/kg ( $\Delta_f H^\circ$ ) <sup>[11]</sup> , -321.7 kJ/mol (enthalpy of form., exptl.) <sup>[3]</sup> , -360.8 kJ/mol (enthalpy of form., calcd., emp.) <sup>[3]</sup> , -270.9 kJ/mol (enthalpy of form., calcd., S-D method) <sup>[3]</sup> , -833.2 <sup>[5]</sup> , 70 kcal/mol ( $Q_f$ ) <sup>[16]</sup> , -189 kcal/kg (enthalpy of form.) <sup>[22]</sup> , -76.91 kcal/mol ( $\Delta H_f^\circ$ , calcd.) <sup>[25]</sup>		
Heat of combustion	$Q_c$ = 1,645 cal/g <sup>[16]</sup>		
	Calcd. (EXPL05 6.04)	Lit. values	Exptl.

$-\Delta_{\text{ex}}U^0$ [kJ kg <sup>-1</sup> ]	5,994	6,488 (calcd., K-J) <sup>[4]</sup> 7,400 <sup>[16]</sup> 1,370 kcal/kg (@ 1.860 g cm <sup>-3</sup> , calcd.) [H <sub>2</sub> O vapor] <sup>[22]</sup>	6,454 [H <sub>2</sub> O (l)] <sup>[5]</sup> 1,378 kcal/kg [H <sub>2</sub> O (g)] <sup>[11]</sup> 6,542 <sup>[14]</sup> 1,378 kcal/kg (@ 1.860 g cm <sup>-3</sup> ) [H <sub>2</sub> O vapor] <sup>[22]</sup>
$T_{\text{ex}}$ [K]	4,199		
$p_{\text{CJ}}$ [GPa]	343		
VoD [m s <sup>-1</sup> ]	8,917 (@ 1.86 g cm <sup>-3</sup> , $\Delta_f H = -313$ kJ mol <sup>-1</sup> )	9,130 (@ 1.86 g cm <sup>-3</sup> (TMD), calcd., R-P method) <sup>[20]</sup>  8,680 (@ 1.86 g cm <sup>-3</sup> (TMD), calcd., Aizenshtadt method) <sup>[20]</sup>  8,990 (@ 1.86 g cm <sup>-3</sup> (TMD), calcd., K-J method) <sup>[20]</sup>  6,050 (@ 1 g cm <sup>-3</sup> , calcd., Kamlet method) <sup>[19]</sup>  8,100 (@ 1.6 g cm <sup>-3</sup> , calcd., Kamlet method) <sup>[19]</sup>  5,540 (@ 1 g cm <sup>-3</sup> , calcd., Urizar method) <sup>[19]</sup>  7,960 (@ 1.6 g cm <sup>-3</sup> , calcd., Urizar method) <sup>[19]</sup>	9,000 (@ 1.98 g cm <sup>-3</sup> ) <sup>[6]</sup>  9,010 (1.86 g cm <sup>-3</sup> ) <sup>[7,21]</sup>  8,100 (@ 1.60 g cm <sup>-3</sup> ) <sup>[17]</sup>  7,950 (@ 1.6 g cm <sup>-3</sup> ) <sup>[19]</sup>  5,500 (@ 1 g cm <sup>-3</sup> ) <sup>[19]</sup>
$V_0$ [L kg <sup>-1</sup> ]	756		697 <sup>[5,9]</sup> 768 <sup>[14]</sup>
$I_{\text{sp}}$ [Ns g <sup>-1</sup> ]	2.52 (calcd., ISPBKW code) <sup>[25]</sup> , 2.49 (calcd., empirical) <sup>[25]</sup>		
Trauzl test [cm <sup>3</sup> , % TNT]	460 mL <sup>[16,24]</sup> , 169% TNT <sup>[18]</sup>		
Ballistic mortar test	144% TNT <sup>[18]</sup>		
Thermal stability	1% mass loss @ 80 °C in 700 h <sup>[16]</sup> , 1% mass loss @ 100 °C in 53 h <sup>[16]</sup>		

	BTNEU <sup>[15]</sup>
Chemical formula	C <sub>5</sub> H <sub>6</sub> N <sub>6</sub> O <sub>13</sub>
Molecular weight [g mol <sup>-1</sup> ]	386.15
Crystal system	Orthorhombic
Space group	Pnn2 (most probable space group)
a [Å]	10.47 ± 0.02
b [Å]	11.25 ± 0.02
c [Å]	5.85 ± 0.01
α [°]	90
β [°]	90
γ [°]	90
V [Å <sup>3</sup> ]	689
Z	2
ρ <sub>calc</sub> [g cm <sup>-3</sup> ]	1.86
T [K]	Not specified

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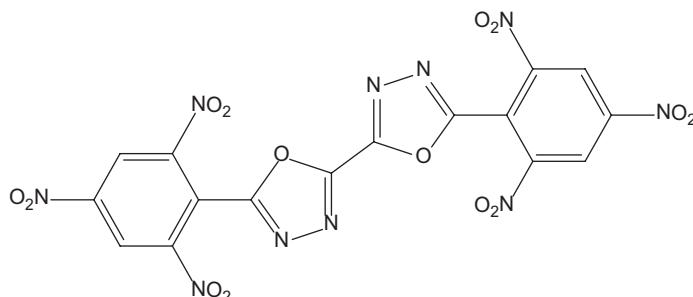
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**5,5'-Bis(2,4,6-trinitrophenyl)-2,2'-bi(1,3,4-oxadiazole)**

Name [German, acronym]: 5,5'-Bis(2,4,6-trinitrophenyl)-2,2'-bi(1,3,4-oxadiazole)  
[TKX-55]

Main (potential) use: Thermally stable explosive

Structural formula:



	TKX-55		
Formula	C <sub>16</sub> H <sub>4</sub> N <sub>10</sub> O <sub>14</sub>		
Molecular mass [g mol <sup>-1</sup> ]	560.26		
Appearance at RT			
IS [J]	5 <sup>[1]</sup>		
FS [N]	>360 <sup>[1]</sup>		
ESD [J]	1.0 <sup>[1]</sup>		
N [%]	25.00		
Ω(CO <sub>2</sub> ) [%]	-57.11		
T <sub>dec.</sub> [°C]	335 (DSC @ 5 °C/min) <sup>[1]</sup>		
ρ [g cm <sup>-3</sup> ]	1.837 (@ 298 K) <sup>[1]</sup>		
Heat of formation	197.6 kJ/mol (ΔH <sup>o</sup> <sub>f</sub> ) <sup>[1]</sup> , 352.7 kJ kg <sup>-1</sup> (ΔH <sup>o</sup> <sub>f</sub> ) <sup>[1]</sup>		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
– Δ <sub>ex</sub> U <sup>o</sup> [kJ kg <sup>-1</sup> ]	4,577		
T <sub>ex</sub> [K]	3,532		
p <sub>C,J</sub> [kbar]	243		

VoD [ $\text{m s}^{-1}$ ]	7,601 (@ 1.837 g $\text{cm}^{-3}$ )	7,548 (@ 1.837 g $\text{cm}^{-3}$ , calcd., CHEETAH v. 8.0) <sup>[2]</sup>	8,230 ± 260 (@ 1.837 g $\text{cm}^{-3}$ ) <sup>[1,2]</sup>
$V_0$ [L $\text{kg}^{-1}$ ]	601		

TKX-55·3C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	
Chemical formula	C <sub>16</sub> H <sub>4</sub> N <sub>10</sub> O <sub>14</sub> ·3C <sub>4</sub> H <sub>8</sub> O <sub>2</sub> <sup>a</sup>
Molecular weight [g mol <sup>-1</sup> ]	824.58
Crystal system	Triclinic
Space group	P-1 (no. 2)
$a$ [\mathring{A}]	6.6985(8)
$b$ [\mathring{A}]	7.7673(6)
$c$ [\mathring{A}]	16.6519(15)
$\alpha$ [°]	98.627(7)
$\beta$ [°]	99.922(9)
$\gamma$ [°]	91.635(8)
$V$ [\mathring{A} <sup>3</sup> ]	842.46(14)
$Z$	1
$\rho_{\text{calc}}$ [g $\text{cm}^{-3}$ ]	1.625
$T$ [K]	227

<sup>a</sup>1,4-Dioxane solvate.

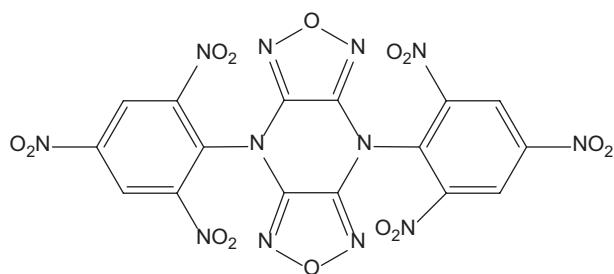
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**4,8-Bis(2,4,6-trinitrophenyl)-4*H*,8*H*-bis([1,2,5]oxadiazolo)[3,4-b:3',4'-e]pyrazine**

Name [German, acronym]: 4,8-Bis(2,4,6-trinitrophenyl)-4*H*,8*H*-bis([1,2,5]oxadiazolo)[3,4-b:3',4'-e]pyrazine

Main (potential) use: Potential new heat-resistant explosive<sup>[1]</sup>

Structural formula:



	<b>4,8-Bis(2,4,6-trinitrophenyl)-4<i>H</i>,8<i>H</i>-bis([1,2,5]oxadiazolo)[3,4-b:3',4'-e]pyrazine</b>		
Formula	$C_{16}H_4N_{12}O_{14}$		
Molecular mass [g mol <sup>-1</sup> ]	588.28		
Appearance at RT	Yellow powder <sup>[1]</sup>		
IS [J]	10 (ZBL-B instrument) <sup>[1]</sup>		
FS [N]	240 (FSKM 10 instrument) <sup>[1]</sup>		
ESD [J]	1 (ESD 2008A electric spark tester) <sup>[1]</sup>		
N [%]	28.57		
$\Omega(CO_2)$ [%]	-54.4		
$T_{dec.}$ [°C]	415 (DSC @ 10 °C/min) <sup>[1]</sup>		
$\rho$ [g cm <sup>-3</sup> ]	1.82 (gas pycnometer @ 25 °C) <sup>[1]</sup>		
Heat of formation	894.1 kJ/mol ( $\Delta H_f$ ) <sup>[1]</sup>		
	Calcd. (EXPL05 6.03)	Lit. values	Exptl.
$-\Delta_{ex}U^\circ$ [kJ kg <sup>-1</sup> ]			
$T_{ex}$ [K]			

$p_{\text{CJ}}$ [kbar]		28.1 GPa (@ 1.82 g cm <sup>-3</sup> , $\Delta H_f = 894.1 \text{ kJ/mol}$ , calcd., K-J) <sup>[1]</sup>	
VoD [m s <sup>-1</sup> ]		7874 (@ 1.82 g cm <sup>-3</sup> , $\Delta H_f = 894.1 \text{ kJ/mol}$ , calcd., K-J) <sup>[1]</sup>	
$V_0$ [L kg <sup>-1</sup> ]			

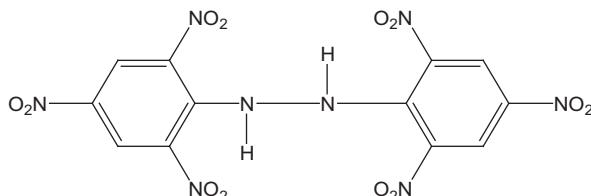
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## 1,2-Bis(2,4,6-trinitrophenyl)hydrazine

Name [German, acronym]: Hexanitrohydrazobenzene, [hexanitrohydrazobenzol, HNHB]

Main (potential) use: Precursor in the synthesis of hexanitrazabenzene<sup>[1]</sup>

Structural formula:



	1,2-Bis(2,4,6-trinitrophenyl)hydrazine		
Formula	C <sub>12</sub> H <sub>6</sub> N <sub>8</sub> O <sub>12</sub>		
Molecular mass [g mol <sup>-1</sup> ]	454.22		
Appearance at RT	Fine crystalline solid <sup>[1]</sup>		
IS [J]	H <sub>50%</sub> = insensitive up to 90 cm (2 kg mass) <sup>[1]</sup>		
FS [N]	insensitive up to load >36 kg (Julius–Peters apparatus, 0/5) <sup>[1]</sup>		
N [%]	24.67		
Ω(CO <sub>2</sub> ) [%]	-52.8		
T <sub>m.p.</sub> [°C]	235–237 <sup>[1]</sup>		
ρ [g cm <sup>-3</sup> ]	1.75 <sup>[1]</sup>		
Heat of formation	11 kJ/mol (ΔH <sub>f</sub> ) <sup>[1]</sup>		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
-Δ <sub>ex</sub> U <sup>0</sup> [kJ kg <sup>-1</sup> ]		2,827 (@ 1.75 g cm <sup>-3</sup> , calcd., LOTUSES) <sup>[1]</sup>	
T <sub>ex</sub> [K]		2,870 (@ 1.75 g cm <sup>-3</sup> , calcd., LOTUSES) <sup>[1]</sup>	
p <sub>CJ</sub> [kbar]		25.26 GPa (@ 1.75 g cm <sup>-3</sup> , calcd., LOTUSES) <sup>[1]</sup>	
VoD [m s <sup>-1</sup> ]		7,360 (@ 1.75 g cm <sup>-3</sup> , calcd., LOTUSES) <sup>[1]</sup>	

$V_0$ [L kg <sup>-1</sup> ]		972 (@ 1.75 g cm <sup>-3</sup> , calcd., LOTUSSES) <sup>[1]</sup>	
Solubility [g/mL]		Recryst. from MeOH <sup>[1]</sup>	

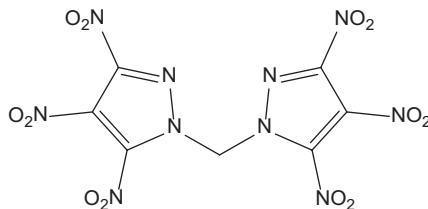
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## Bis(3,4,5-trinitropyrazoly)methane

Name [German, acronym]: Bis(3,4,5-trinitropyrazoly)methane [BTNPM]

Main (potential) use: High explosive

Structural formula:



	<b>BTNPM</b>		
Formula	$C_7H_2N_{10}O_{12}$		
Molecular mass [g mol <sup>-1</sup> ]	418.2		
Appearance at RT			
IS [J]	4 <sup>[1]</sup>		
FS [N]	144 <sup>[1]</sup>		
ESD [J]	0.1 <sup>[1]</sup>		
N [%]	33.50		
$\Omega(CO_2)$ [%]	-11.48		
$T_{dec.}$ [°C]	205 (DSC @ 5 °C/min) <sup>[1]</sup>		
$\rho$ [g cm <sup>-3</sup> ]	1.934 (@ 298 K) <sup>[1]</sup>		
Heat of formation	378.6 kJ/mol ( $\Delta H_f^\circ$ ) <sup>[1]</sup> , 976.8 kJ kg <sup>-1</sup> ( $\Delta H_f^\circ$ ) <sup>[1]</sup>		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl. (est. LASEM method)
$-\Delta_{ex}U^\circ$ [kJ kg <sup>-1</sup> ]	6191		
$T_{ex}$ [K]	4572		
$p_{C_J}$ [kbar]	401		
VoD [m s <sup>-1</sup> ]	9,293 (@ 1.934 g/cc)	9,276 (@ TMD, calcd., CHEETAH v. 8.0) <sup>[2]</sup>	$9,910 \pm 310^{[2]}$
$V_0$ [L kg <sup>-1</sup> ]	711		

	<b>BTNPM</b>
Chemical formula	C <sub>7</sub> H <sub>2</sub> N <sub>10</sub> O <sub>12</sub>
Molecular weight [g mol <sup>-1</sup> ]	418.19
Crystal system	Monoclinic
Space group	P2 <sub>1</sub> /n (no. 14)
<i>a</i> [Å]	8.6118(3)
<i>b</i> [Å]	16.5734(5)
<i>c</i> [Å]	29.794(1)
$\alpha$ [°]	90
$\beta$ [°]	95.938(1)
$\gamma$ [°]	90
<i>V</i> [Å <sup>3</sup> ]	4229.6(2)
<i>Z</i>	12
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.970
<i>T</i> [K]	173

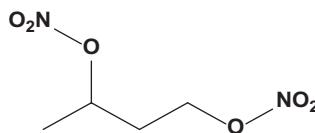
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## Butanediol dinitrate

Name [German, acronym]: 1,3-Butanediol dinitrate, 1,3-butylene glycol dinitrate, dinitrobutylene glycol [1,3-butylenglykoldinitrat]

Main (potential) use: Suggested for use in nonfreezing dynamites<sup>[7]</sup>

Structural formula:



	<b>Butanediol dinitrate</b>	
Formula	$\text{C}_4\text{H}_8\text{N}_2\text{O}_6$	
Molecular mass [g mol <sup>-1</sup> ]	180.12	
Appearance at RT	Oily liquid @ 15 °C <sup>[4]</sup> , colorless liquid <sup>[6,7]</sup> , oily liquid <sup>[8]</sup>	
N [%]	15.55	
$\Omega(\text{CO}_2)$ [%]	-53.3	
$T_{\text{m.p.}}$ [°C]	-20 <sup>[3]</sup> , -20 (freezing point) <sup>[8]</sup>	
$T_{\text{dec.}}$ [°C]	Sudden heating causes deflagration <sup>[7]</sup>	
$\rho$ [g cm <sup>-3</sup> ]	$1.352 \pm 0.06$ (@ 293.15 K) <sup>[1]</sup> , 1.32 <sup>[3]</sup> , sp. gr. = 1.32 <sup>[4,8]</sup> , $d^{20}_{4} = 1.3167$ <sup>[5]</sup> , sp. gr. = 1.32 (@ 15 °C) <sup>[7]</sup> , $d^{20}_{4} = 1.3167$ (1,3-isomer) <sup>[8]</sup> , $d^{20}_{4} = 1.3061$ (2,3-isomer) <sup>[8]</sup>	
Heat of formation	-243.4 kJ/mol ( $\Delta_f H^\circ$ , calcd.) <sup>[2]</sup> , -1,351.3 kJ kg <sup>-1</sup> ( $\Delta_f H^\circ$ , calcd.) <sup>[2]</sup> , -274.1 kJ/mol (enthalpy of form., exptl.) <sup>[9]</sup> , -331.6 kJ/mol (enthalpy of form., calcd., emp.) <sup>[9]</sup>	
	Calcd. (K-J)	Exptl.
$-\Delta_{\text{ex}} U^\circ$ [kJ kg <sup>-1</sup> ]		
$T_{\text{ex}}$ [K]		
$p_{\text{C-J}}$ [GPa]		
VoD [m s <sup>-1</sup> ]		
$V_0$ [L kg <sup>-1</sup> ]		

Trauzl test [cm <sup>3</sup> , % TNT]	Expansion 75% NG <sup>[4]</sup> , 460 cm <sup>3</sup> <sup>[3,8]</sup> , 370 cm <sup>3</sup> (10 g) <sup>[6]</sup> , ~240 cc expansion from 75% butanediol dinitrate/25% Kieselguhr mixture <sup>[7]</sup>
5 s explosion <i>T</i> [°C] Explosion <i>T</i> [°C]	Sudden heating causes deflagration <sup>[7]</sup>
Volatility	More volatile than NG <sup>[4]</sup> , highly volatile <sup>[8]</sup>
Viscosity [cP]	$\eta_{20} = 6.00^{[5]}$ , $\eta_{20} = 6.00$ (1,3-isomer) <sup>[8]</sup> , $\eta_{20} = 4.7$ (2,3-isomer) <sup>[8]</sup>
Dipole moment [D]	3.74 (pure, 1,3-isomer) <sup>[8]</sup> , 3.45 (soln. in benzene, 1,3-isomer) <sup>[8]</sup> , 4.72 (pure, 2,3-isomer) <sup>[8]</sup> , 4.12 (soln. in benzene, 2,3-isomer) <sup>[8]</sup>
Dielectric constant	$\epsilon_{20} = 18.85$ (1,3-isomer) <sup>[8]</sup> , $\epsilon_{20} = 28.84$ (2,3-isomer) <sup>[8]</sup>
Solubility [g/mL]	Insoluble in H <sub>2</sub> O <sup>[6]</sup> , soluble in most solvents suitable for NG <sup>[6]</sup>
Refractive index	$n^{20}_{\infty} = 1.43259$ (1,3-isomer) <sup>[8]</sup> , $n^{20}_{\infty} = 1.42754$ (2,3-isomer) <sup>[8]</sup>

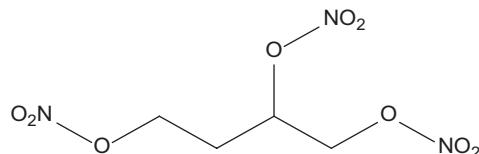
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## Butanetriol trinitrate

Name [German, acronym]: Butane-1,2,4-triyl trinitrate,  $\alpha,\beta,\gamma$ -trihydroxybutane trinitrate, 1,2,4-butanetriol trinitrate, butanetriol trinitrate, nitrobutanetriol, nitrutone trioxide [1,2,4-butanetrioltrinitrat, BTTN, BTN]

Main (potential) use: Plasticizer<sup>[1]</sup>, explosive plasticizer for cellulose<sup>[7]</sup>, double-base propellants, nitroglycerine replacement in explosives and propellants<sup>[14]</sup>, gelatinizer for nitrocellulose<sup>[14]</sup>, semicommercial-scale production during World War-II<sup>[15]</sup>, double-base propellants or high-energy propellants (mixed with NG)<sup>[5]</sup>, liquid propellant or liquid explosive<sup>[5]</sup>

Structural formula:



	<b>BTTN</b>
Formula	$\text{C}_4\text{H}_7\text{N}_3\text{O}_9$
Molecular mass [g mol <sup>-1</sup> ]	241.11
Appearance at RT	Yellow oil <sup>[7]</sup> , light yellow liquid <sup>[14]</sup> , clear yellow liquid <sup>[5]</sup>
IS [J]	1 Nm <sup>[2,17]</sup> , 4.7 cm <sup>[8]</sup> , 11.4 <sup>[10]</sup> , 58 cm (2 kg mass, 20 mg sample, B.M.) <sup>[7,13]</sup> , ≤1 in (1 lb mass, P.A.) <sup>[7,13]</sup> , $H_{50} = 25$ cm <sup>[16]</sup> , 58 cm (2 kg hammer) <sup>[5]</sup>
N [%]	17.43
$\Omega(\text{CO}_2)$ [%]	-16.6
$T_{\text{m.p.}}$ [°C]	-2.7 <sup>[10]</sup> , -5.9 (endotherm peak onset, DSC @ 10 °C/min) <sup>[12]</sup> , -5.8 to -3.2 (visual mpt., purified) <sup>[12]</sup> , -7.6 to -2.8 (visual mpt., as received) <sup>[12]</sup> , -27 <sup>[14,16]</sup> , -2.7 (freezing point) <sup>[5]</sup>
$T_{\text{dec.}}$ [°C]	176 (TGA midpoint) <sup>[17]</sup>
$T_{\text{glass transition}}$ [°C]	-68.0 (DSC (glass transition ( $T_{\text{g1/2}}$ ) @ 10 °C/min)) <sup>[12]</sup> , -68.5 (DSC (glass transition ( $T_{\text{g1/2}}$ ) @ 10 °C/min), rerun) <sup>[12]</sup> , -65 (DSC midpoint) <sup>[17]</sup>
$\rho$ [g cm <sup>-3</sup> ]	1.52 (@ 298.15 K) <sup>[3,8,13]</sup> , 1.520 (@ 20 °C) <sup>[14]</sup> , 1.52 <sup>[7,16,18]</sup> , 1.52 (loading density) <sup>[7]</sup> , sp. gr. = 1.52 <sup>[5]</sup>

Heat of formation	−406 kJ/mol ( $\Delta_f H^\circ$ ) <sup>[4]</sup> , −1,683 kJ kg <sup>−1</sup> ( $\Delta_f H^\circ$ , ICT thermochemical database) <sup>[4]</sup> , −1,682 J/g ( $\Delta_f H^\circ$ ) <sup>[6]</sup> , 368 cal/g <sup>[14]</sup> , −1,683.9 kJ/kg <sup>[18]</sup> , −414.2 kJ/mol (enthalpy of form., exptl.) <sup>[6]</sup> , −402.1 kJ/mol (enthalpy of form., calcd., emp.) <sup>[6]</sup> , −97.04 kcal/mol ( $\Delta H_f^\circ$ ) <sup>[19]</sup>		
Heat of combustion	2,167 cal/g <sup>[14]</sup> , $Q_c = 2,168 \text{ cal/g}^{[7,13]}$ , $\Delta H_c = 9,071 \text{ J/g}^{[16]}$		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{ex} U^\circ$ [kJ kg <sup>−1</sup> ]		6,022 (calcd., ICT code) <sup>[4,17]</sup> 1,457 cal/g <sup>[7,13]</sup> 1,440 kcal/kg <sup>[15]</sup> $\Delta_e H = 6,021 \text{ J/g}^{[16]}$ 6,025 (constant volume) [H <sub>2</sub> O (g)] <sup>[5]</sup> 5,941 (constant volume) [H <sub>2</sub> O (l)] <sup>[5]</sup>	6,096 <sup>[7]</sup> 1,457 cal/g <sup>[7]</sup> 6,025 J/g [H <sub>2</sub> O (g)] <sup>[10]</sup> 5,941 J/g [H <sub>2</sub> O (l)] <sup>[10]</sup> 6,153 <sup>[11]</sup> 6,022 J/g [H <sub>2</sub> O (l)] <sup>[2]</sup> 5,551 J/g [H <sub>2</sub> O (g)] <sup>[2]</sup> 1,458 cal/g <sup>[14]</sup>
$T_{ex}$ [K]		3,917 (calcd., ICT code) <sup>[4]</sup>	
$p_{C_J}$ [GPa]		139.0 MPa (calcd., ICT code) <sup>[4]</sup>	
VoD [m s <sup>−1</sup> ]			
$V_0$ [L kg <sup>−1</sup> ]		634 cm <sup>3</sup> /g (without H <sub>2</sub> O @ 25 °C) <sup>[17]</sup> 840 [H <sub>2</sub> O (l)] <sup>[5]</sup>	836 <sup>[2,9]</sup> 840 <sup>[7,13]</sup> 865 <sup>[11]</sup>
$I_{sp}$ [Ns g <sup>−1</sup> ]	2.59 (calcd., ISPBKW code) <sup>[19]</sup> , 2.56 (calcd., empirical) <sup>[19]</sup>		

Sand test [g]	48.6 g sand crushed (200 g bomb) <sup>[7,13]</sup> , 103% TNT <sup>[14]</sup> , 49 g (cf. 51.5 g for NG or 47 g for TNT) <sup>[14]</sup>
Ballistic mortar test	
Initiation efficiency	0.20 g LA minimum detonating charge <sup>[7]</sup> , 0.10 g tetryl minimum detonating charge <sup>[7]</sup>
5 s explosion $T$ [ $^{\circ}$ C]	dec. @ 230 $^{\circ}$ C <sup>[7,13]</sup> , 230 <sup>[5,14]</sup>
100 $^{\circ}$ C heat test [% mass loss]	1.5% mass loss in first 48 h <sup>[7,13]</sup> , 1.2% mass loss in second 48 h <sup>[7,13]</sup> , no explosion in 100 h <sup>[7,13]</sup>
Vacuum stability test [cm <sup>3</sup> /h]	2.33 cc/g/16 h @ 100 $^{\circ}$ C <sup>[13]</sup> , 2.33 cc/40 h @ 100 $^{\circ}$ C <sup>[7]</sup>
Vapor pressure [atm @ $^{\circ}$ C]	~50% that of NG <sup>[5]</sup>
Volatility	Less volatile than NG <sup>[15]</sup> , 46.0 mg·cm <sup>2</sup> ·h <sup>-1</sup> (@ 60 $^{\circ}$ C) <sup>[7,16]</sup> , ~50% that of NG <sup>[5]</sup>
Viscosity [cP]	59 (@ 25 $^{\circ}$ C) <sup>[7,13]</sup> , 62 (@ 20 $^{\circ}$ C) <sup>[14]</sup> , 2.2 times that of NG <sup>[5]</sup>
Solubility [g/mL]	0.08g in 100 g H <sub>2</sub> O @ 20 $^{\circ}$ C <sup>[5,7]</sup> , 0.15 g in 100 g H <sub>2</sub> O @ 60 $^{\circ}$ C <sup>[5,7]</sup> , soluble in Et <sub>2</sub> O <sup>[7]</sup> , slightly soluble in water <sup>[14]</sup> , miscible with EtOH, Et <sub>2</sub> O, acetone and 2:1 Et <sub>2</sub> O/EtOH <sup>[14]</sup> , miscible with Et <sub>2</sub> O, EtOH, ketone and other organic solvents <sup>[5]</sup>
Hygroscopicity	0.14 % @ 100 $^{\circ}$ F in 24 h @ 95 % RH <sup>[7]</sup> , 0.04% @ 65% humidity <sup>[5]</sup>
Refractive index	$n_D^{20} = 1.4738^{[7,14]}$

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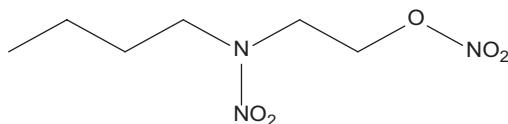
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## N-Butyl-N-(2-nitroxyethyl)nitramine

Name [German, acronym]: N-Butyl-N-(2-nitroxyethyl)nitramine, [1-(*N*-butyl-nitramino)-ethan-2-ol] nitrate, *n*-butyl nitroso ethyl nitramine, *N*-(2-nitroxyethyl) butylnitramine [*N*-butyl-2-nitrosoethyl-nitramin, BuNENA]

Main (potential) use: Plasticizer for propellant formulations<sup>[1]</sup>

Structural formula:



	BuNENA		
Formula	$\text{C}_6\text{H}_{13}\text{N}_3\text{O}_5$		
Molecular mass [g mol <sup>-1</sup> ]	207.19		
Appearance at RT	Liquid <sup>[6]</sup>		
IS [J]	>100 cm (5 kg drop-weight, BAM) <sup>[4]</sup> , 6 Nm <sup>[9]</sup>		
<i>N</i> [%]	20.28		
$\Omega(\text{CO}_2)$ [%]	-104.3		
$T_{\text{m.p.}}$ [°C]	-9.1 <sup>[2,4]</sup> , -9.9 (freezing point) <sup>[2]</sup> , -27 to -28 <sup>[5]</sup> , <-9 <sup>[6]</sup>		
$T_{\text{glass transition}}$ [°C]	-48 (DSC midpoint) <sup>[9]</sup> , -82.5 (DSC @ 10 °C/min) <sup>[7]</sup>		
$T_{\text{dec.}}$ [°C]	153 (onset) with maximum at 191 (DSC @ 5 °C/min) <sup>[4]</sup> , 210 (exo, DSC) <sup>[5]</sup> , 208 (DSC @ 10 °C/min, 99.7% purity) <sup>[8]</sup> , 212 (DSC @ 10 °C/min, 99.6% purity) <sup>[8]</sup> , 211 (DSC @ 10 °C/min, 98.9% purity) <sup>[8]</sup> , 211 (DSC @ 10 °C/min, 99.2% purity) <sup>[8]</sup> , 211 (DSC @ 10 °C/min, 99.4% purity) <sup>[8]</sup> , 152 (TGA midpoint) <sup>[9]</sup>		
$\rho$ [g cm <sup>-3</sup> ]	$1.242 \pm 0.06$ (@ 293 K) <sup>[3]</sup> , 1.22 <sup>[1,4,7]</sup> , 1.21 <sup>[5,6]</sup>		
Heat of formation	-192.47 kJ/mol ( $\Delta_f H^\circ$ ) <sup>[1,4]</sup> , -928.94 kJ kg <sup>-1</sup> ( $\Delta_f H^\circ$ ) <sup>[1]</sup> , 259 kJ/mol ( $\Delta_f H$ ) <sup>[5]</sup> , -46 cal/mol ( $\Delta_f H$ ) <sup>[6]</sup> , -192.5 kJ/mol (enthalpy of form., exptl.) <sup>[10]</sup> , -199.4 kJ/mol (enthalpy of form., calcd., emp.) <sup>[10]</sup>		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.

$-\Delta_{\text{ex}}U^{\circ} [\text{kJ kg}^{-1}]$		259 cal/g ( $Q_{\text{ex}}$ @ 0.20 g cm $^{-3}$ , calcd., Blake code) <sup>[6]</sup>  3,573 J/g [H <sub>2</sub> O (l)] (ICT thermodynamic code) <sup>[9]</sup>	
$T_{\text{ex}} [\text{K}]$			
$p_{\text{CJ}} [\text{GPa}]$			
VoD [m s $^{-1}$ ]			
$V_0 [\text{L kg}^{-1}]$		1,045 cm $^3$ /g (without H <sub>2</sub> O, @ 25 °C) <sup>[9]</sup>	

Thermal stability	23 wt.% mass loss on heating in N <sub>2</sub> stream up to 120 °C <sup>[9]</sup>
Abel test (82.2 °C) [min]	5.5 (99.7% purity) <sup>[8]</sup> , 6 (99.6% purity) <sup>[8]</sup> , 5.5 (98.9% purity) <sup>[8]</sup> , 5.5 (99.2% purity) <sup>[8]</sup> , 5 (99.4% purity) <sup>[8]</sup>

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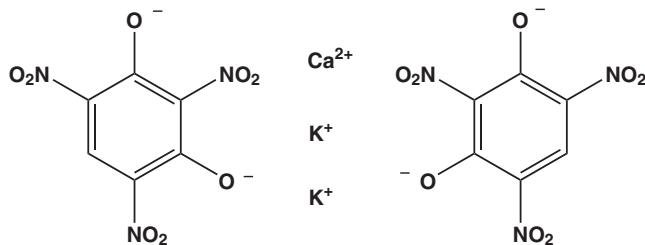
# C

## Calcium potassium styphnate

Name [German, acronym]: Calcium potassium styphnate, calcium potassium bis(2,4,6-trinitro-*m*-phenylene dioxide)  
[kalium-calcium-styphnat, castyp]

Main (potential) use: Heavy metal-free primary explosive in priming mixtures for small-caliber ammunition primers<sup>[1]</sup>

Structural formula:



	Calcium potassium styphnate	
Formula	$C_{12}H_2CaK_2N_6O_{16}$	
Molecular mass [g mol <sup>-1</sup> ]	604.45	
Appearance at room temperature (RT)		
IS [J]	>0.2 Nm <sup>[1]</sup> , 3 <sup>[2]</sup> , 3 (basic potassium calcium styphnate) <sup>[2]</sup>	
FS [N]	>0.5 <sup>[1]</sup> , 9 <sup>[2]</sup> , 9 (basic potassium calcium styphnate) <sup>[2]</sup>	
ESD [J]	>0.0004 <sup>[1]</sup>	
N [%]	13.90	
$\Omega(CO_2)$ [%]	-23.8	
$T_{dec.}$ [°C]	345 <sup>[2]</sup> , 340 (basic potassium calcium styphnate) <sup>[2]</sup>	
	Calcd. (K-J)	Exptl.
$-\Delta_{ex}U^\circ$ [kJ kg <sup>-1</sup> ]		
$T_{ex}$ [K]		

$p_{\text{CJ}}$ [GPa]		
VoD [m s <sup>-1</sup> ]		
$V_0$ [L kg <sup>-1</sup> ]		

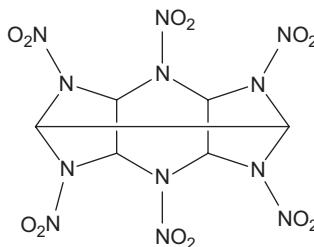
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**ε-CL-20**

Name [German, acronym]: 2,4,6,8,10,12-Hexanitro-2,4,6,8,10,12-hexaazaisowurtzitane,  
 5,2,6-(iminomethenimino)-1H-imidazo[4,5-b]pyrazine,  
 ε-hexanitrohexaazaisowurtzitane, 2,4,6,8,10,12-hexanitro-  
 2,4,6,8,10,12-hexaazatetracyclo[5.5.0.0<sup>3,11</sup>.0<sup>5,9</sup>]-dodecane  
 [(ε-CL-20) (HNIW)]\*

Main (potential) use: Secondary (high) explosive

Structural formula:



\* Crystal lattice of α-CL-20 is stabilized by addition of H<sub>2</sub>O to unit cell, and X-ray diffraction shows H<sub>2</sub>O cavity occupancy of 17–50%. Therefore, α-CL-20 should be considered a hydrate of CL-20.<sup>[28]</sup>

	<b>HNIW</b>
Formula	C <sub>6</sub> H <sub>6</sub> N <sub>12</sub> O <sub>12</sub>
Molecular mass [g mol <sup>-1</sup> ]	438.19
Appearance at RT	white solid
IS [J]	3 (<100 µm), 11.90 (sound) <sup>[1,5,34]</sup> , 5.38 (first reaction) <sup>[1,5,34]</sup> , 4 Nm <sup>[2]</sup> , 4 <sup>[4]</sup> , 11.90 <sup>[7,8]</sup> , H <sub>50</sub> = 28 cm (2 kg hammer) <sup>[24]</sup> , H <sub>50</sub> = 14 cm <sup>[25]</sup> , 2 (ground CL-20) <sup>[37]</sup> , 2 (coarse CL-20) <sup>[37]</sup> , 1 Nm (ε-CL-20) <sup>[40]</sup> , 3 (commercial-grade CL-20, 100–150 µm particle size, BAM) <sup>[41]</sup> , H <sub>50</sub> = 28 cm (2 kg hammer, E <sub>d50</sub> = 5.6 J) <sup>[50]</sup> , H <sub>50</sub> = 26.8 cm (5 kg mass, 30 mg sample, GJB-772A-97 standard method 601.2) <sup>[52]</sup> , 25 cm (15 µm particle size) <sup>[71]</sup> , 55 cm (0.095 µL particle size) <sup>[71]</sup> , 9–11 cm (ERL) <sup>[23,30]</sup> , 1–3.5 cm (ABL) <sup>[23,30]</sup> , 19–36 in (TC apparatus) <sup>[23]</sup> , CL-20 deflagrated strongly at all drop heights ≥0.15 m, but no deflagration with 0.10 m drop height (glass-anvil drop weight machine, max. drop height = 1.3 m) <sup>[29]</sup> , 14 cm (β-, 2.5 kg mass, type 12 tool, 35 mg pressed sample) <sup>[27,65]</sup> , 12–16 cm (ε-, Aerojet, 2.5 kg mass, type 12 tool, 35 mg pressed sample) <sup>[27,65]</sup> , 17 cm (ε-, Thiokol, 2.5 kg mass, type 12 tool, 35 mg pressed sample) <sup>[27,65]</sup> , 21 cm (ε-, Thiokol ground to 3–5 µm, 2.5 kg mass, type 12 tool, 35 mg pressed sample) <sup>[27,65]</sup>

	<p>Drop energy for 50% initiation probability<sup>[17]</sup>: 6.15 for <math>\beta</math>-HNIW (25 mg sample, Julius-Peters apparatus)<sup>[17]</sup>, 5.38 for <math>\epsilon</math>-HNIW (25 mg sample, Julius-Peters apparatus)<sup>[17]</sup>,</p> <p>Size, density and sensitivity of CL-20 crystalline particles (C-CL20 = commonly used CL-20; D-CL20 = desensitized CL-20)<sup>[20]</sup>.</p> <table border="1"> <thead> <tr> <th>Material</th><th>Mean size <math>d_{50}</math> (<math>\mu\text{m}</math>)</th><th>Average crystal <math>\rho</math> @ 20 °C (<math>\text{g cm}^{-3}</math>)</th><th><math>H_{50}</math> (cm of go and no go; hammer: 2 kg, sample: 30 mg)</th></tr> </thead> <tbody> <tr> <td>C-CL-20</td><td>99.5</td><td><math>2.0290 \pm 0.0005</math></td><td><math>15.0 \pm 0.1</math></td></tr> <tr> <td>D-CL-20</td><td>71.5</td><td><math>2.0380 \pm 0.0003</math></td><td><math>42.6 \pm 0.1</math></td></tr> </tbody> </table> <p><math>H_{50}</math> of micro/nano-CL-20 crystals (2 kg mass, 30 mg sample, WL-1-type apparatus)<sup>[54]</sup>:</p> <table border="1"> <thead> <tr> <th>CL-20 sample</th><th>Particle size (<math>\mu\text{m}</math>)</th><th><math>H_{50}</math> (cm)</th></tr> </thead> <tbody> <tr> <td>Raw material</td><td>100</td><td>18.6</td></tr> <tr> <td>After grinding</td><td>1–5</td><td>23.2</td></tr> <tr> <td>After solvent/nonsolvent recryst.</td><td>80</td><td>45.7</td></tr> <tr> <td>Assembled crystal #1</td><td>40</td><td>57.4</td></tr> <tr> <td>Assembled crystal #2</td><td>4</td><td>66.9</td></tr> <tr> <td>Assembled crystal #3</td><td>240</td><td>39.4</td></tr> </tbody> </table> <p><math>H_{50} = 38.5 \pm 2.9</math> cm (raw <math>\epsilon</math>-HNIW, HGZ-1 apparatus, 2.5 kg mass)<sup>[61]</sup>,  <math>H_{50} = 44.2 \pm 4.1</math> cm (raw nano-<math>\epsilon</math>-HNIW, HGZ-1 apparatus, 2.5 kg mass)<sup>[61]</sup></p> <p>Nano-CL-20, values at which 50% samples explode, 2 kg mass, Julius-Peter apparatus, CL-20 purity = 99% (&gt;95% <math>\epsilon</math>-polymorph)<sup>[62]</sup>:</p> <table border="1"> <thead> <tr> <th>Average particle size (<math>\mu\text{m}</math>)</th><th>Impact (cm)</th></tr> </thead> <tbody> <tr> <td>15</td><td>25</td></tr> <tr> <td>4</td><td>32</td></tr> <tr> <td>1</td><td>40</td></tr> <tr> <td>0.095</td><td>55</td></tr> </tbody> </table> <p><math>H_{50} = 13.6</math> cm (2.5 kg mass, 35 mg sample, raw CL-20, average particle size, <math>D_{50} = 15.96 \mu\text{m}</math>, HGZ-1 machine)<sup>[64]</sup>, <math>H_{50} = 13.6</math> cm (2.5 kg mass, 35 mg sample, nano-CL-20 produced by ball-milling, average particle size, <math>d_{50} = 200 \text{ nm}</math>, HGZ-1 machine)<sup>[64]</sup>, 5.0 (15 <math>\mu\text{m}</math> crystal size)<sup>[70]</sup>, 6.4 (4 <math>\mu\text{m}</math> crystal size)<sup>[70]</sup>, 8.0 (1 <math>\mu\text{m}</math> crystal size)<sup>[70]</sup>, 11.0 (0.095 <math>\mu\text{m}</math> crystal size)<sup>[70]</sup>, <math>A_{d1} = 100\%</math>, <math>A_{d2} = 100\%</math><sup>[16]</sup>, <math>H_{50\%} = 13.6 \pm 0.11</math> cm (2.5 kg hammer, micron-sized CL-20, <math>d_{50} = 40\text{--}60 \mu\text{m}</math>)<sup>[73]</sup>, <math>H_{50\%} = 29.4 \pm 0.09</math> cm (2.5 kg hammer, nanosized CL-20)<sup>[73]</sup></p>	Material	Mean size $d_{50}$ ( $\mu\text{m}$ )	Average crystal $\rho$ @ 20 °C ( $\text{g cm}^{-3}$ )	$H_{50}$ (cm of go and no go; hammer: 2 kg, sample: 30 mg)	C-CL-20	99.5	$2.0290 \pm 0.0005$	$15.0 \pm 0.1$	D-CL-20	71.5	$2.0380 \pm 0.0003$	$42.6 \pm 0.1$	CL-20 sample	Particle size ( $\mu\text{m}$ )	$H_{50}$ (cm)	Raw material	100	18.6	After grinding	1–5	23.2	After solvent/nonsolvent recryst.	80	45.7	Assembled crystal #1	40	57.4	Assembled crystal #2	4	66.9	Assembled crystal #3	240	39.4	Average particle size ( $\mu\text{m}$ )	Impact (cm)	15	25	4	32	1	40	0.095	55
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	<p><math>DH_{50} = 36.7 \text{ cm}, 39.7 \text{ cm}</math> (as-made RX-39-AC formulation (<math>\epsilon</math>-HNIW/Estane, 95.8/4.2 wt.%), 2.5 kg mass, type 12 tool)<sup>[82]</sup>, <math>DH_{50} = 37.6 \text{ cm}</math> (heated for 24 h @ 100 °C RX-39-AC formulation (<math>\epsilon</math>-HNIW/Estane, 95.8/4.2 wt.%), 2.5 kg mass, type 12 tool)<sup>[82]</sup>)</p> <p>2 kg mass, BAM, max. height at which explosion from at least <math>1/6</math> trials was observed (no relationship between crystal shape and IS was observed)<sup>[85]</sup>:</p> <table border="1"> <thead> <tr> <th>CL-20 crystallized with addition of crystal growth modifier</th><th>Impact sensitivity (J)</th><th>CL-20 crystallized with addition of crystal growth modifier</th><th>Impact sensitivity (J)</th></tr> </thead> <tbody> <tr> <td>None</td><td>2</td><td>Diethylene glycol</td><td>4</td></tr> <tr> <td>1,2,5-Triacetoxypentane</td><td>4</td><td>Formic acid</td><td>4</td></tr> <tr> <td>Glycine</td><td>3</td><td>Triacetin</td><td>4</td></tr> <tr> <td>Ethylene glycol</td><td>5</td><td>Ethyl alcohol</td><td>4</td></tr> <tr> <td>Acetone</td><td>4</td><td></td><td></td></tr> </tbody> </table> <p>(see additional table at the end of section)</p>	CL-20 crystallized with addition of crystal growth modifier	Impact sensitivity (J)	CL-20 crystallized with addition of crystal growth modifier	Impact sensitivity (J)	None	2	Diethylene glycol	4	1,2,5-Triacetoxypentane	4	Formic acid	4	Glycine	3	Triacetin	4	Ethylene glycol	5	Ethyl alcohol	4	Acetone	4		
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Ethylene glycol	5	Ethyl alcohol	4																						
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FS [N]	<p>96 (&lt;100 <math>\mu\text{m}</math>), 54<sup>[2]</sup>, 28<sup>[4]</sup>, 69<sup>[6-8]</sup>, <math>p_{\text{fr,LL}} = 150 \text{ MPa}</math><sup>[16]</sup>, 11–15 kg (BAM)<sup>[23]</sup>, 110 psi @ 2 ft/s (ABL)<sup>[23]</sup>, 10–15 kg (BAM)<sup>[30]</sup>, 110 psi @ 2 ft/s – 110 psi @ 4 ft/s (ABL)<sup>[30]</sup>, 6.4 kg (<math>\beta</math>-, Julius-Peters app., <math>1/10</math> positive)<sup>[27,65]</sup>, 6.4–7.2 kg (<math>\epsilon</math>-, aerojet, Julius-Peters app., <math>1/10</math> positive)<sup>[27,65]</sup>, 6.4 kg (<math>\epsilon</math>-, Thiokol, Julius-Peters app., <math>1/10</math> positive)<sup>[27,65]</sup>, 6.2 kg (<math>\epsilon</math>-, Thiokol ground to 3–5 <math>\mu\text{m}</math>, Julius-Peters app., <math>1/10</math> positive)<sup>[27,65]</sup>, 40 (ground CL-20)<sup>[37]</sup>, 80 (coarse CL-20)<sup>[37]</sup>, 108<sup>[40]</sup>, 84 (commercial-grade CL-20, 100–150 <math>\mu\text{m}</math> particle size, BAM)<sup>[41]</sup>, <math>P = 100\%</math> (explosion probability, angle of pendulum = 90 °, rel. pressure = 3.92 MPa)<sup>[52]</sup>, <math>P = 62\%</math> (raw <math>\epsilon</math>-HNIW, <math>P</math> = explosive probability, WM-1 apparatus, <math>45 \pm 1^\circ</math>, 2.45 MPa)<sup>[61]</sup>, <math>P = 60\%</math> (nano-<math>\epsilon</math>-HNIW, <math>P</math> = explosive probability, WM-1 apparatus, <math>45 \pm 1^\circ</math>, 2.45 MPa)<sup>[61]</sup>, 6.4 kg (15 <math>\mu\text{m}</math> particle size)<sup>[71]</sup>, no reaction (0.095 <math>\mu\text{L}</math> particle size)<sup>[71]</sup></p> <p>Nano-CL-20, Julius-Peters apparatus, 35 mg sample, CL-20 purity = 99%, &gt;95% <math>\epsilon</math>-polymorph<sup>[62]</sup>:</p> <table border="1"> <thead> <tr> <th>Average particle size (<math>\mu\text{m}</math>)</th><th>FS (kg)</th></tr> </thead> <tbody> <tr> <td>15</td><td>6.4</td></tr> <tr> <td>4</td><td>8</td></tr> <tr> <td>1</td><td>No reaction</td></tr> <tr> <td>0.095</td><td>No reaction</td></tr> </tbody> </table>	Average particle size ( $\mu\text{m}$ )	FS (kg)	15	6.4	4	8	1	No reaction	0.095	No reaction														
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	<p>82% (probability of explosion, 20 mg sample, <math>80 \pm 1^\circ</math>, 2.45 MPa, raw CL-20, average particle size, <math>d_{50} = 15.96 \mu\text{m}</math>, WM-1 machine)<sup>[64]</sup>, 66% (probability of explosion, 20 mg sample, <math>80 \pm 1^\circ</math>, 2.45 MPa, nano-CL-20 produced by ball-milling, average particle size, <math>d_{50} = 200 \text{ nm}</math>, WM-1 machine)<sup>[64]</sup>, 64 (50% load, 15 <math>\mu\text{m}</math> crystal size)<sup>[70]</sup>, 80 (50% load, 4 <math>\mu\text{m}</math> crystal size)<sup>[70]</sup>, no reaction (50% load, 1 <math>\mu\text{m}</math> crystal size)<sup>[70]</sup>, no reaction (50% load, 0.095 <math>\mu\text{m}</math> crystal size)<sup>[70]</sup>, 88% (sliding friction test, <math>80^\circ</math> angle, 2.45 MPa, micron-sized CL-20, <math>d_{50} = 40\text{--}60 \mu\text{m}</math>)<sup>[73]</sup>, 66% (sliding friction test, <math>80^\circ</math> angle, 2.45 MPa, nanosized CL-20)<sup>[73]</sup></p> <p><math>^1/_{10}</math> @ 11.6 kg (as-made RX-39-AC formulation (<math>\epsilon</math>-HNIW/Estane, 95.8/4.2 wt.%), BAM)<sup>[82]</sup>, <math>^1/_{10}</math> @ 11.2 kg (heated for 24 h @ <math>100^\circ\text{C}</math> RX-39-AC formulation (<math>\epsilon</math>-HNIW/Estane, 95.8/4.2 wt.%), BAM)<sup>[82]</sup></p> <p>BAM, lower limit of sensitivity was the lowest load at which explosion was observed in at least <math>^1/_{10}</math> trials<sup>[85]</sup>:</p> <table border="1"> <thead> <tr> <th>CL-20 crystallized with addition of crystal growth modifier</th><th>Friction sensitivity (N)</th><th>CL-20 crystallized with addition of crystal growth modifier</th><th>Friction sensitivity (N)</th></tr> </thead> <tbody> <tr> <td>None</td><td>54</td><td>Diethylene glycol</td><td>158</td></tr> <tr> <td>1,2,5-Triacetoxypentane</td><td>126</td><td>Formic acid</td><td>126</td></tr> <tr> <td>Glycine</td><td>119</td><td>Triacetin</td><td>142</td></tr> <tr> <td>Ethylene glycol</td><td>158</td><td>Ethyl alcohol</td><td>126</td></tr> <tr> <td>Acetone</td><td>126</td><td></td><td></td></tr> </tbody> </table> <p>(see additional data at the end of section)</p>	CL-20 crystallized with addition of crystal growth modifier	Friction sensitivity (N)	CL-20 crystallized with addition of crystal growth modifier	Friction sensitivity (N)	None	54	Diethylene glycol	158	1,2,5-Triacetoxypentane	126	Formic acid	126	Glycine	119	Triacetin	142	Ethylene glycol	158	Ethyl alcohol	126	Acetone	126		
CL-20 crystallized with addition of crystal growth modifier	Friction sensitivity (N)	CL-20 crystallized with addition of crystal growth modifier	Friction sensitivity (N)																						
None	54	Diethylene glycol	158																						
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ESD [J]	<p>0.10 (&lt;100 <math>\mu\text{m}</math>), 4.70<sup>[1,3]</sup>, 462.0 mJ<sup>[3]</sup>, depends on size<sup>[23]</sup>, 0.5 to &gt;8<sup>[30]</sup>, no reaction (<math>\beta</math>-, 10 tries @ 1 J with <math>510 \Omega</math> in line resistance)<sup>[27,65]</sup>, no reaction (<math>\epsilon</math>-, Aerojet, 10 tries @ 1 J with <math>510 \Omega</math> in line resistance)<sup>[27,65]</sup>, no reaction (<math>\epsilon</math>-, Thiokol ground to 3–5 <math>\mu\text{m}</math>, 10 tries @ 1 J with <math>510 \Omega</math> in line resistance)<sup>[27,65]</sup>, 0.45 (commercial-grade CL-20, 100–150 <math>\mu\text{m}</math> particle size, BAM)<sup>[41]</sup>, <math>V_{50} = 4.64 \text{ kV}</math> (bulk CL-20, JGY-50-type apparatus)<sup>[51]</sup>, <math>E_{50} = 0.106</math> (bulk CL-20, JGY-50-type apparatus)<sup>[51]</sup>, &gt;5600 mJ</p> <p>(old equipment), 5,600 mJ (medium particle size of 169 <math>\mu\text{m}</math>, new equipment)<sup>[57]</sup>, 45 (15 <math>\mu\text{m}</math> crystal size)<sup>[70]</sup>, 49 (4 <math>\mu\text{m}</math> crystal size)<sup>[70]</sup>, 49 (1 <math>\mu\text{m}</math> crystal size)<sup>[70]</sup>, 60 (0.095 <math>\mu\text{m}</math> crystal size)<sup>[70]</sup>, 45 (15 <math>\mu\text{m}</math> particle size)<sup>[71]</sup>, 60 (0.095 <math>\mu\text{L}</math> particle size)<sup>[71]</sup>, <math>^0/_{10}</math>, no go (as-made RX-39-AC formulation (<math>\epsilon</math>-HNIW/Estane, 95.8/4.2 wt.%), 1.0 J, 500 <math>\Omega</math> resistance with pigmented mylar film oversample)<sup>[82]</sup>, <math>^0/_{10}</math>, no go (as-made RX-39-AC formulation (<math>\epsilon</math>-HNIW/Estane, 95.8/4.2 wt.%), 1.0 J, 500 <math>\Omega</math> resistance with pigmented mylar film oversample).<sup>[82]</sup></p> <p>ESD sensitivity of CL-20 as a function of spark duration (50% ignition level, spark duration = time from breakdown of the sample until 99% of the spark energy has been discharged, 15 shot Bruceton staircase technique with Pearson current monitor)<sup>[59]</sup>:</p>																								

	Damping resistor (Ω)	Capacitor (nF)	Voltage (kV)	Capacitor energy eq. (1) (mJ)	Measured spark energy eq. (2) (mJ)	Spark duration (μs)	Time to max. light output (μs)
0	5.1	8.04	165	36	1.80	2.08	
3.4	5.1	8.40	180	17	0.86	0.87	
10	16	7.83	490	24	0.64	0.75	
48	31	7.18	799	15	3.1	2.31	
100	199	7.89	6190	43	>17.0	5.65	
1000	350	7.90	10920	37	No rxn.	No rxn.	

Nano-CL-20, RD and D apparatus (Zbrojovka Indet., Vsetin, Czech Rep.), voltage of capacitor = 11 kV, CL-20 purity = 99%, >95% ε-polymorph<sup>[62]</sup>:

Average particle size (μm)	Electrostatic (J)
15	45
4	49
1	49
0.095	60

$N$ [%]	38.36
$\Omega(\text{CO}_2)$ [%]	-10.95
$T_{\text{m.p.}}$ [°C]	513 K <sup>[65,74]</sup> , 260 (with dec.) <sup>[68]</sup> , 260 ( $\beta$ -, needle-shaped prism crystals, with dec.) <sup>[80]</sup> , 260 ( $\alpha$ -, hemihydrate, rhombic crystals, with dec.) <sup>[80]</sup>
$T_{\text{b.p.}}$ [°C]	862 K <sup>[65]</sup> , 861.8 K (est., $T_{\text{nbp}}$ , Stein–Brown method) <sup>[74]</sup>
$T_{\text{p.t.}}$ [°C]	160 (phase transition), 205 ( $\epsilon$ - → $\gamma$ -) (single crystal, nanocalorimetric curve, thermal cycle @ 1400 °C/s) <sup>[19]</sup> , $\gamma$ - is thermodynamically most stable phase @ $T > 64$ °C <sup>[27]</sup> and $\beta$ - and $\epsilon$ - slowly convert to $\gamma$ -phase <sup>[27]</sup> , 165 (larger endotherm, $\epsilon$ - → $\gamma$ -transition), 220 (smaller endotherm, $\alpha$ - (contaminant) → $\gamma$ -) (DSC @ 10 °C/min, ε-CL-20) <sup>[27]</sup> , 64 ( $\epsilon$ - → $\gamma$ -transition) <sup>[28]</sup> , the pressure-induced conversion of $\gamma$ - → $\zeta$ - is a reversible transition @ 0.7 GPa <sup>[28]</sup> , phase transition to $\zeta$ - only observed from $\gamma$ - <sup>[28]</sup> , 135 to ~226 ( $\beta$ -phase transition) <sup>[28]</sup> , $\epsilon$ - converted in range ~157–176 ( $\epsilon$ -crystals @ 10 °C/min) <sup>[28]</sup> , nonsolvated $\alpha$ -samples crumbled in the range of the first endo response (~160 °C); crystals embedded in silicone partly gave vigorous bubbling during fragmentation and conversion and is consistent with H <sub>2</sub> O loss. Visual changes in the same crystals @ 200–220 °C (second endo temperature range) were inconclusive in determining phase change (hot-stage microscopy) <sup>[28]</sup> , high pressure $\zeta$ -phase can be produced in reversible transition from $\gamma$ -phase <sup>[28]</sup> , CL-20 recrystallizes from dichloromethane but reverts back to a different polymorph assumed to be ε-CL-20 <sup>[37]</sup>

	DSC measurements, 1–3 mg samples, perforated Al pans <sup>[28]</sup> :		
Polymorph	Scan rate (°C/min)	Endotherm (max., °C)	
α-	10	172	
	5	169	
	2	166	
Dehydrated α- (vacuum dry)	10	181	
α- (H <sub>2</sub> O wetted)	10	172	
	5	156	
	2	162–167	
β-	10	146	
γ-	10	None observed	
ε-	40	182	
	20	173	
	10	167–171	
	5	165	
	2	163	
	1	160	
	0.5	159	
<p>164.2 (endo, onset), 171.1 (endo, peak max.) (fast, quantitative, irreversible solid ε- → solid γ-phase transition, DSC @ 0.5–10 K/min)<sup>[31]</sup>, cooling and heating again of γ- shows no phase transition<sup>[31]</sup>, 140 (slow ε- → γ-transition after 20 h storage of ε- @ 140 °C, that is, &lt;164 °C)<sup>[31]</sup>, 220–226 (β-crystals cracked and evolved gas)<sup>[28]</sup>, 230 (β-crystals blackened)<sup>[28]</sup>, ~220 (gas evolved in ε-crystals)<sup>[28]</sup></p> <p>β-CL-20 obtained by dissolving ε-CL-20 in ethyl acetate, then soln. rapidly injected under N<sub>2</sub> atmosphere into CHCl<sub>3</sub> and seeded with a few β-CL-20 crystals<sup>[43]</sup>, γ-CL-20 obtained by dissolving ε-CL-20 in acetic acid @ 115 °C and allowing solvent to boil off until material crystallized from soln., sample was repeatedly washed with H<sub>2</sub>O until neutral.<sup>[43]</sup></p> <p>Influence on the purity of CL-20 on the initial ε-→γ-phase transition temperature of CL-20 determined using in situ powder X-ray diffraction<sup>[46]</sup>:</p>			
Average particle size (μm)	Mean density (g cm <sup>-3</sup> )	Purity (%)	Initial phase transition temperature (°C)
65.2	2.0309	94.20	145
59.7	2.0324	95.53	150
62.3	2.0334	96.37	150
59.5	2.0349	98.25	155
55.7	2.0382	99.62	160

Phase-transition status of CL-20 at different temperatures and isothermal time (samples heated @ 0.1 °C/s from ambient temperature to target temperature and then scanned for 5 min at constant temperature, powder X-ray diffraction data was collected every 30 min for 8 h)<sup>[46]</sup>:

Isothermal time (min)	Phase status of CL-20				
	@ 145 °C	@ 150 °C	@ 155 °C	@ 160 °C	@ 165 °C
30	ε-	ε-	ε-	ε-	ε-, γ-
60	ε-	ε-	ε-	ε-, γ-	ε-, γ-
120	ε-	ε-	ε-, γ-	ε-, γ-	ε-, γ-
180	ε-	ε-	ε-, γ-	ε-, γ-	ε-, γ-
240	ε-	ε-, γ-	ε-, γ-	ε-, γ-	ε-, γ-
300	ε-	ε-, γ-	ε-, γ-	ε-, γ-	ε-, γ-
360	ε-	ε-, γ-	ε-, γ-	ε-, γ-	ε-, γ-
420	ε-	ε-, γ-	ε-, γ-	ε-, γ-	ε-, γ-
480	ε-	ε-, γ-	ε-, γ-	ε-, γ-	γ-
		Weak γ-phase appears and gradually increases	Weak γ-phase appears and gradually increases	Weak γ-phase appears and gradually increases	Weak γ-phase appears and gradually increases; entire phase transition to γ-phase occurs

Effect of solvent and crystallization conditions on the phase transitions of CL-20 (@ 20 °C, ethyl acetate or acetone soln. saturated with CL-20, s = slow addition (1 mL/min) of antisolvent, f = fast addition (15 mL/min) of antisolvent, R = instant reverse addition which is the addition of CL-20 saturated ethyl acetate or acetone soln. to an antisolvent instantaneously); an unstable solvate of CL-20 is obtained in acetone soln. if an alkane is used as the antisolvent @ 20 °C and from this the β-form can be obtained in air<sup>[45]</sup>:

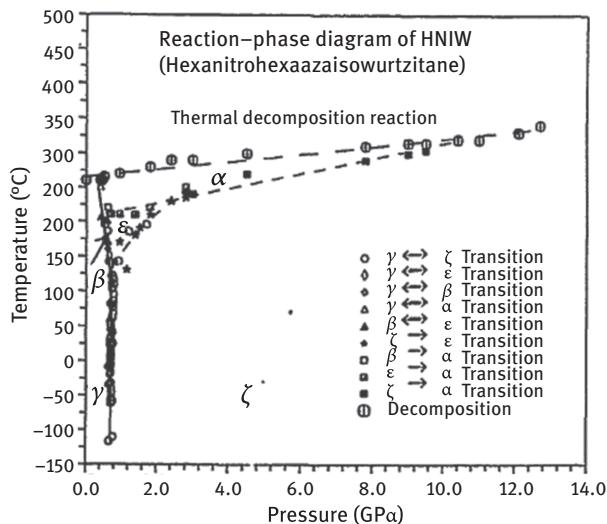
	Antisolvent	$\mu \times 10^{-30}$ (C.m)	Polarity	Polymorphic transformation in soln.			
	Hexane	0	0	$\varepsilon^-$	$\varepsilon^-$	$\beta^- \rightarrow \varepsilon^-$	Solvate
	Heptane	0	0	$\varepsilon^-$	$(\beta^- + \varepsilon^-) \rightarrow \varepsilon^-$	$\beta^- \rightarrow \varepsilon^-$	Solvate
	Petroleum ether	0	0.01	$\varepsilon^-$	$\varepsilon^-$	$\beta^- \rightarrow \varepsilon^-$	Solvate
	Decalin	0	0	$\varepsilon^-$	$\varepsilon^-$	$\beta^- \rightarrow \varepsilon^-$	Solvate
	Octane	0	0	$\varepsilon^-$	$\beta^- \rightarrow \varepsilon^-$	$\beta^- \rightarrow \varepsilon^-$	Solvate
	Cyclohexane	0	0.10	$(\beta^- + \varepsilon^-) \rightarrow \varepsilon^-$	$(\beta^- + \varepsilon^-) \rightarrow \varepsilon^-$	$\beta^- \rightarrow \varepsilon^-$	Solvate
	$\text{CCl}_4$	0	1.60	$(\beta^- + \varepsilon^-) \rightarrow \varepsilon^-$	$\beta^- \varepsilon^-$	$\beta^- \rightarrow \varepsilon^-$	$\beta^- \rightarrow \varepsilon^-$
	Benzene	0	3.00	$\varepsilon^-$	$\varepsilon^-$	$\beta^- \rightarrow \varepsilon^-$	$\beta^- \rightarrow (\alpha^- + \varepsilon^-) \rightarrow \varepsilon^-$
	Toluene	1.2	2.40	$\varepsilon^-$	$\varepsilon^-$	$\beta^- \rightarrow \varepsilon^-$	$\beta^- \rightarrow \varepsilon^-$
	$\text{CH}_2\text{Cl}_2$	3.8	3.40	$\beta^- \rightarrow \varepsilon^-$	$\beta^- \rightarrow \varepsilon^-$	$\beta^- \rightarrow \varepsilon^-$	$\beta^- \rightarrow \varepsilon^-$
	$\text{CHCl}_3$	3.84	4.40	$\beta^- \rightarrow \varepsilon^-$	$\beta^- \rightarrow \varepsilon^-$	$\beta^- \rightarrow \varepsilon^-$	$\beta^- \rightarrow \varepsilon^-$
	1,1,2-Trichloroethane	5.17		$\beta^- \rightarrow \varepsilon^-$	$\beta^- \rightarrow \varepsilon^-$	$\beta^- \rightarrow \varepsilon^-$	$\beta^- \rightarrow \varepsilon^-$
	$\text{H}_2\text{O}$	6.18	10.2	$\alpha^-$	$\alpha^-$	$\alpha^-$	$\alpha^-$

Effect of temperature on the polymorphic transformation in various solvents<sup>[45]</sup>:

Solvent/antisolvent	$T$ (°C)	Polymorphic transformation
Acetone/1,1,2-trichloroethane	65	$\beta^- \rightarrow \varepsilon^-$
	70	$\beta^- \rightarrow (\varepsilon^- + \gamma^-) \rightarrow \gamma^-$
	75	$\beta^- \rightarrow \varepsilon^-$
Acetone/heptane	65	$\beta^- \rightarrow \varepsilon^-$
	70	$\beta^- \rightarrow (\varepsilon^- + \gamma^-)$
	75	$\beta^- \rightarrow (\varepsilon^- + \gamma^-) \gamma^- \rightarrow$
	80	$\beta^- \rightarrow \varepsilon^-$
Ethyl acetate/1,1,2-trichloroethane	75	$\beta^- \rightarrow \varepsilon^-$
	80	$\beta^- \rightarrow (\varepsilon^- + \gamma^-) \gamma^- \rightarrow$
	85	$\beta^- \rightarrow \varepsilon^-$
Ethyl acetate/heptane	75	$\beta^- \rightarrow \varepsilon^-$
	80	$\beta^- \rightarrow \varepsilon^- \rightarrow (\varepsilon^- + \gamma^-)$
	85	$\beta^- \rightarrow (\varepsilon^- + \gamma^-) \rightarrow \gamma^-$

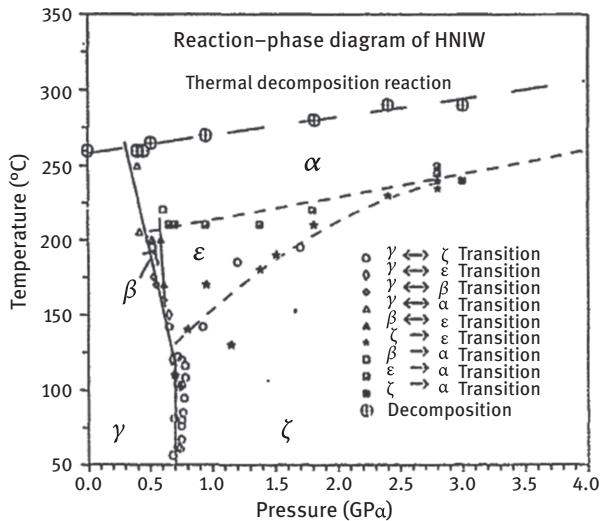
	<p>Large crystal (1–2 mm) of <math>\alpha</math>-HNIW can be obtained by slow evaporation of the solvent from a <math>\gamma</math>-HNIW solution in ethyl acetate<sup>[53]</sup></p> <p>The <math>\epsilon \rightarrow \gamma</math>-phase transition is usually accompanied by loss of water since crystals of <math>\epsilon</math>-HNIW dried under normal conditions usually contain an admixture of water<sup>[53]</sup>. The <math>\epsilon \rightarrow \gamma</math>-phase transition starts after full dehydration has occurred at elevated temperatures and finishes at initial stages of HNIW decomposition<sup>[53]</sup></p> <p><math>\epsilon</math>-CL-20 is the thermodynamically stable polymorph under ambient conditions<sup>[65]</sup>, <math>\beta</math>-CL-20 converts to <math>\gamma</math>-CL-20 @ 185 °C<sup>[65]</sup>, heating <math>\gamma</math>-CL-20 to 230 °C converts it to <math>\delta</math>-CL-20 – was initially reported but is now thought to correspond to a structural modification instead<sup>[65]</sup>, <math>\delta</math>-CL-20 is only stable @ elevated pressures<sup>[65]</sup>, <math>\zeta</math>-CL-20 present @ high pressure during reversible phase transition of <math>\gamma</math>-CL-20 @ <math>0.7 \pm 0.05</math> GPa<sup>[65]</sup>, <math>\epsilon</math>-CL-20 is stable under ambient pressure to <math>T \sim 120</math> °C<sup>[65]</sup> but phase transition to <math>\gamma</math>-CL-20 occurs @ 125 °C and <math>\gamma</math>-CL-20 is stable up to thermal dec. &lt;150 °C<sup>[65]</sup></p> <p><math>T_p = 162 \pm 1</math> °C (<math>\epsilon \rightarrow \gamma</math>, solid-solid phase transition, DSC @ 5 °C/min, pinhole pan, N<sub>2</sub>, Turcotte)<sup>[65]</sup>, formation of <math>\alpha</math>-/<math>\beta</math>-CL-20 mainly depends on soln. used for recryst. or precipitation of CL-20: <math>\alpha</math>-CL-20 formed on precip. of CL-20 from sulfolane soln. using CHCl<sub>3</sub> (Wardle)<sup>[65]</sup>. <math>\beta</math>-CL-20 present on recryst. of CL-20 form benzene soln. (Wardle)<sup>[65]</sup>. <math>\gamma</math>-CL-20 synthesized by nitrolysis of diformyl derivative using nitric acid<sup>[65]</sup></p> <p><math>\alpha</math>- = orthorhombic (high-temperature–high-pressure phase), <math>\beta</math>- = orthorhombic (high-pressure phase), <math>\gamma</math>- = monoclinic (stable ambient phase), <math>\epsilon</math>- = monoclinic (high-temperature–high-pressure phase), <math>\zeta</math>- = monoclinic (high-pressure phase); solid–solid phase transitions among the known polymorphs of CL-20 determined as a function of temperature and pressure<sup>[72]</sup>:</p>				
Transition	Reversibility	Press. region (GPa)	Temp. region (°C)	Technique	Transition boundary
$\gamma/\alpha$ -	Rev.	0.40–0.55 > 180	FTIR	Neg.	
$\gamma/\beta$ -	Rev.	0.55–0.62	160–180	FTIR	Neg.
$\gamma/\epsilon$ -	Rev.	0.62–0.70	120–160	FTIR,OPLM	neg.
$\gamma/\zeta$ -	Rev.	0.70	−125–120	FTIR, OPLM,EDXD	No
$\beta/\alpha$ -	Nonrev.	0.4–0.55	190	FTIR	Pos.
$\beta/\epsilon$ -	Nonrev.	140–170	FTIR	Undeter.	
$\epsilon/\alpha$ -	Nonrev.	0.6–2.8	190–220	FTIR	Pos.
$\zeta/\epsilon$ -	Nonrev.	0.70–2.8	130–180	FTIR	Pos.
$\zeta/\alpha$ -	Nonrev.	2.8–10	190–230	FTIR	Pos.

Reaction/phase diagram for  $\gamma$ -HNIW showing the measured stability fields for the five solid-phase polymorphs ( $\alpha$ -,  $\beta$ -,  $\gamma$ -,  $\varepsilon$ -,  $\zeta$ -) from  $-150$  to  $-320$   $^{\circ}\text{C}$  and up to  $14.0$  GPa, data from ref. [72]:



**Fig. 4:** Reaction–phase diagram of HNIW: pressure versus temperature<sup>[72]</sup>.

Reaction–phase diagram for  $\gamma$ -HNIW showing the measured stability fields for the five solid-phase polymorphs ( $\alpha$ -,  $\beta$ -,  $\gamma$ -,  $\varepsilon$ -,  $\zeta$ -) from  $-150$  to  $320$   $^{\circ}\text{C}$  and up to  $14.0$  GPa, showing an enlarged view of the region from  $50$  to  $320$   $^{\circ}\text{C}$  and up to  $4.0$  GPa, data from ref. [72]:



**Fig. 5:** Reaction–phase diagram of HNIW: pressure versus temperature<sup>[72]</sup>.

$\zeta$ -Phase exists @ RT above 0.7 GPa<sup>[75]</sup>

Four stable polymorphic forms under ambient conditions:  $\alpha$ -,  $\beta$ -,  $\gamma$ -,  $\epsilon$ -, as well as a labile form ( $\zeta$ ) which exists only at high pressures<sup>[80]</sup>, the  $\alpha$ -form contains centrosymmetric cavities which if all are singly occupied forms a semihydrate,<sup>[80]</sup> whereas if only half of the cavities are filled by water molecules then a 0.25 hydrate is formed<sup>[80]</sup>, ~185 (heating  $\beta$ -form between thin glass discs converts to  $\gamma$ -form)<sup>[80]</sup>, >185 (heating  $\beta$ -form above 185 °C forms  $\delta$ - @ 230 °C which has been shown to be most likely a different crystalline form of the  $\gamma$ -polymorph and not the crystalline form of a different polymorph)<sup>[80]</sup>, six polymorphs from  $\alpha$ - to  $\zeta$ - have been described<sup>[81]</sup>, thermodynamic stability order:  $\epsilon$ - (most stable polymorph @ RT) >  $\gamma$ - (monoclinic,  $P2_1/c$ ) >  $\alpha$ -hydrate (orthorhombic,  $Pbca$ ) >  $\beta$ - (orthorhombic,  $Pb2_1a$ )<sup>[83]</sup>, the existence of multiple  $\alpha$ -hydrate phases complicates the phase diagram<sup>[83]</sup>,  $\delta$ - (high  $T$  phase appearing immediately before dec., hot-stage microscopy, DSC, hexagonal crystal phase but not isolated in pure form)<sup>[83]</sup>,  $\zeta$ - from high pressure, occurs due to reversible transition from  $\gamma$ -phase<sup>[83]</sup>, solvents possessing –OH groups (e.g. EtOH, H<sub>2</sub>O) preferentially stabilize  $\alpha$ -polymorph and slow its conversion @ ambient  $T$  to the  $\epsilon$ - (more stable) polymorph<sup>[83]</sup>, order of soln. indicates stability order:  $\epsilon$ - >  $\gamma$ - >  $\alpha$ - >  $\beta$ -<sup>[83]</sup>

Variation of solvent and temperature with  $\beta$ -phase conversions  
(FEFO = bis(fluorofinitroethyl)formal, poly(caprolactone)triol with average MW = 300)<sup>[83]</sup>:

Solvent	$T$ (°C)	Time heated (days)	Final polymorph
None	55	10	Beta
FEFO	55	4	Gamma
FEFO	42	5	Gamma
FEFO	38	4	Beta
1-Butanol	38	4	Gamma
Poly(caprolactone)triol (dry)	40	4	Beta
Poly(caprolactone)triol (dry)	38	10	Beta + alpha
Poly(caprolactone)triol (wet)	37	7	Alpha

The lowest  $T$  for  $\alpha$ -phase conversion is controlled by extent of hydration of  $\alpha$ -phase –  $\alpha$ -hydrate stirred in xylenes converts to  $\gamma$ -phase @ 95 °C (close to bpt. of H<sub>2</sub>O) which is proposed to correspond to disruption of  $\alpha$ -crystal lattice followed by phase transition to  $\gamma$ -phase<sup>[83]</sup>, significant equilibrium time below the 64 °C  $\epsilon$ - →  $\gamma$ -transition allows  $\alpha$ -hydrate to easily convert to  $\epsilon$ -, while dehydrated  $\alpha$ -seeded with epsilon in dry solvent does not<sup>[83]</sup>, the most thermodynamically stable  $\alpha$ -phase at a given  $T$  should be the most hydrated one<sup>[83]</sup>

Maximum endothermic responses as a function of scan speed, solid–solid phase transition by DSC and TA/TGA, 1–3 mg samples placed in crimped, perforated Al pans (\* = no endotherm observed; <sup>†</sup> = corresponds to  $\beta\text{-} \rightarrow \alpha$ , but observed first in wet  $\beta$ -contaminated  $\alpha$ -samples; <sup>‡</sup> = faint due to overlap with exothermic onset)<sup>[84]</sup>:

Polymorph	Scan rate ( $^{\circ}\text{C}/\text{min}$ )	Endotherm max. $T$ ( $^{\circ}\text{C}$ )
Alpha	10	172
	5	169
	2	166
Dehydrated alpha	10	181
$\text{H}_2\text{O}$ -wetted alpha	10	172      203 <sup>†</sup>
	5	156      203 <sup>†</sup>
	2	162–167      203 <sup>†,‡</sup>
Beta	10	146
Gamma	10	*
Epsilon	40	182
	20	173
	10	167–171
	5	165
	2	163
	1	160
	0.5	159

$\alpha$ - and  $\varepsilon$ -CL-20 transform completely into the  $\gamma$ -state before dec. therefore the kinetic data for any CL-20 modification characterizes the thermal behavior of  $\gamma$ -CL-20 formed at the very early stages of thermolysis (IR spectroscopy)<sup>[83]</sup>, the thermal phase transitions  $\alpha\text{-} \rightarrow \gamma$ - and  $\varepsilon\text{-} \rightarrow \gamma$ - precede the thermal dec. of  $\alpha$ -CL-20 and  $\varepsilon$ -CL-20<sup>[83]</sup>,  $\varepsilon$ - is the most thermodynamically stable polymorph @ RT (solvated equilibration conversion studies)<sup>[84]</sup>,  $64 \pm 1$  ( $\varepsilon\text{-} \rightarrow \gamma$  in solvents)<sup>[84]</sup>, thermodynamic stability order:  $\varepsilon\text{-} > \gamma\text{-} > \alpha\text{-} > \beta\text{-}$  (initial diffusion-limited solvent work in FEFO)<sup>[84]</sup>, a high  $T$  endotherm in DSC was observed for wet  $\beta$ -contaminated  $\alpha$ -samples which probably corresponds to an earlier reported  $\delta$ -phase; this conversion was  $\beta\text{-} \rightarrow \gamma$ - (FTIR), no  $\delta$ -phase was isolated<sup>[84]</sup>,  $64$  ( $\varepsilon\text{-} \rightarrow \gamma$ )<sup>[84]</sup>, the pressure-induced conversion of  $\gamma\text{-} \rightarrow \zeta$ - is a reversible transition @ ~0.7 GPa (FTIR)<sup>[84]</sup>, the transition to  $\zeta$ - is not seen from any polymorph except  $\gamma$ -<sup>[84]</sup>

$T_{\text{dec.}} \text{ [}^{\circ}\text{C}]$	<p>224 (DSC @ 5 °C/min), 480 K (DTA @ 5 °C/min)<sup>[5,34]</sup>, 315<sup>[4]</sup>, 340 (single crystal, nanocalorimetric curve, thermal cycle @ 1400 °C/s)<sup>[19]</sup> 220 (exo, DSC @ 10 °C/min, ε-CL-20)<sup>[27]</sup>, 218.9 (exo, onset), 232.5 (exo, peak max., dec. of γ-polymorph) (DSC @ 0.5–10 K/min)<sup>[31]</sup>, 218.87 ± 0.43 (calcd. onset T of dec., T at max. heat flow = 232. 36 ± 0.18 °C, max. heat flow = 3.75 ± 0.17 kW/mol, heat of dec. = 1133.9 ± 29.4 kJ/mol; DSC of ε-CL-20 (resp. γ-CL-20) @ 2 K/min, Ar atmosphere, Al sample pans with pierced lids, mean values from 10 runs, 0.669–0.945 mg sample size)<sup>[31]</sup>, quantitative dec. of ε- @ <math>T &gt; 210</math> °C but also thermal dec. at lower <math>T</math> shown by isothermal TGA<sup>[31]</sup>, 216 (dec. onset)<sup>[35]</sup>, 255.1 (DSC @ 10 °C/min, 3 MPa)<sup>[36]</sup>, 255.4 (DSC @ 10 °C/min, 1 MPa)<sup>[36]</sup>, 254.2 (DSC @ 10 °C/min, 0.1 MPa)<sup>[36]</sup>, under linear heating (heating rate @ 2.4 °C/min) noticeable dec. of α-HNIW &gt; 170 °C and ignition @ 216 °C<sup>[47]</sup>, <math>484 &lt; T_{\text{max.}} = 513 &lt; 529</math> K (DSC, drilled-Al crucible, @ 5 K/min)<sup>[49]</sup>, <math>493 &lt; T_{\text{max.}} = 508 &lt; 509</math> K (mass loss = 82.4%, TG Alumina opened crucible @ 5 K/min)<sup>[49]</sup>, 228 (onset), 248 (peak max.), 260 (end of dec.) (DSC @ 10 °C/min, CL-20 shows single-stage dec., purity &gt;99%, &gt;95% ε-polymorph, nanoparticles)<sup>[62]</sup>, 213<sup>[65]</sup></p> <p>DSC measurements, 1–3 mg samples, perforated Al pans; DSC and TA/TGA, 1–3 mg samples placed in crimped, perforated Al pans<sup>[84]</sup>:</p> <table border="1"> <thead> <tr> <th>Polymorph</th><th>Scan rate (°C/min)</th><th>Exotherm (onset, °C)</th><th>Exotherm (max., °C)</th></tr> </thead> <tbody> <tr> <td>α-</td><td>10</td><td>210</td><td>247</td></tr> <tr> <td></td><td>5</td><td>205</td><td>244</td></tr> <tr> <td></td><td>2</td><td>202</td><td>233</td></tr> <tr> <td>Dehydrated α- (vacuum dry)</td><td>10</td><td>210</td><td>253</td></tr> <tr> <td>α- (H<sub>2</sub>O wetted)</td><td>10</td><td>210</td><td>247</td></tr> <tr> <td></td><td>5</td><td>204</td><td>244</td></tr> <tr> <td></td><td>2</td><td>203</td><td>233</td></tr> <tr> <td>β-</td><td>10</td><td>210</td><td>246</td></tr> <tr> <td>γ-</td><td>10</td><td>210</td><td>249</td></tr> <tr> <td>ε-</td><td>40</td><td>—</td><td>—</td></tr> <tr> <td></td><td>20</td><td>—</td><td>—</td></tr> <tr> <td></td><td>10</td><td>210</td><td>249</td></tr> <tr> <td></td><td>5</td><td>—</td><td>—</td></tr> <tr> <td></td><td>2</td><td>—</td><td>—</td></tr> <tr> <td></td><td>1</td><td>—</td><td>—</td></tr> <tr> <td></td><td>0.5</td><td>—</td><td>—</td></tr> </tbody> </table>	Polymorph	Scan rate (°C/min)	Exotherm (onset, °C)	Exotherm (max., °C)	α-	10	210	247		5	205	244		2	202	233	Dehydrated α- (vacuum dry)	10	210	253	α- (H <sub>2</sub> O wetted)	10	210	247		5	204	244		2	203	233	β-	10	210	246	γ-	10	210	249	ε-	40	—	—		20	—	—		10	210	249		5	—	—		2	—	—		1	—	—		0.5	—	—
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	1	—	—																																																																		
	0.5	—	—																																																																		

	Commercial-grade CL-20, 100–150 µm particle size <sup>[41]</sup> :				
	Method	Heating rate (°C/min)	Atmosphere	Onset dec. (°C)	Max. dec. (°C)
	DTA	10	N <sub>2</sub>	215	233
	DTA	2	N <sub>2</sub>	202	220
	DTA	10	Air	209	232
	DSC	10	N <sub>2</sub>	216	239
	DSC	2	N <sub>2</sub>	205	223
	DSC	10	Air	217	238
	$T_{\text{peak}} = 519.54 \text{ K}$ (raw $\epsilon$ -HNIW, DSC, floating N <sub>2</sub> atmosphere, @ 10 °C/min) <sup>[61]</sup> , $T_{\text{peak}} = 508.68 \text{ K}$ (nano- $\epsilon$ -HNIW, DSC, floating N <sub>2</sub> atmosphere, @ 10 °C/min) <sup>[61]</sup>				
	230.03 (exo, peak max., DSC @ 5 °C/min, N <sub>2</sub> , nano-CL-20 produced by ball milling, average particle size ( $d_{50}$ ) = 200 nm) <sup>[64]</sup> , 236.66 exo, peak max., (DSC @ 10 °C/min, N <sub>2</sub> , nano-CL-20 produced by ball milling, average particle size ( $d_{50}$ ) = 200 nm) <sup>[64]</sup> , 239.61 (exo, peak max., DSC @ 15 °C/min, N <sub>2</sub> , nano-CL-20 produced by ball milling, average particle size ( $d_{50}$ ) = 200 nm) <sup>[64]</sup> , 243.42 (exo, peak max., DSC @ 20 °C/min, N <sub>2</sub> , nano-CL-20 produced by ball milling, average particle size ( $d_{50}$ ) = 200 nm) <sup>[64]</sup> , 235.12 (exo, peak max., DSC @ 5 °C/min, N <sub>2</sub> , raw-CL-20, average particle size ( $d_{50}$ ) = 15.96 µm) <sup>[64]</sup> , 241.80 (exo, peak max., DSC @ 10 °C/min, N <sub>2</sub> , raw-CL-20, average particle size ( $d_{50}$ ) = 15.96 µm) <sup>[64]</sup> , 245.32 (exo, peak max., DSC @ 15 °C/min, N <sub>2</sub> , raw-CL-20, average particle size ( $d_{50}$ ) = 15.96 µm) <sup>[64]</sup> , 247.50 (exo, peak max., DSC @ 20 °C/min, N <sub>2</sub> , raw-CL-20, average particle size ( $d_{50}$ ) = 15.96 µm) <sup>[64]</sup>				
	Observed temperature/pressure parameters for HNIW thermal decomposition at a moderate rate (1–2 min), indicating the decomposing HNIW phase <sup>[72]</sup> :				
	Polymorph	Decomposition			
		Temperature (°C)	Pressure (GPa)		
	γ-	260	0.0–0.4		
	α-	260–280	0.40–10.0		
	ζ-	280–340	10.0–14.0		

$\rho$ [g cm <sup>-3</sup> ]	2.08 (@ 100 K), 2.018 (gas pycnometer @ 298 K), 2.04 (crystalline) <sup>[4,38]</sup> , 1.981 ( $\alpha$ -, crystalline, density gradient method) <sup>[11]</sup> , 1.985 ( $\beta$ -, crystalline, density gradient method) <sup>[11]</sup> , 1.916 ( $\gamma$ -, crystalline, density gradient method) <sup>[11]</sup> , 2.044 ( $\epsilon$ -, crystalline, density gradient method) <sup>[11]</sup> , 2.044 (@ TMD) <sup>[11,23,35]</sup> , 1.92 ( $\gamma$ ) <sup>[22]</sup> , 1.97 ( $\alpha$ ) <sup>[22]</sup> , 1.99 ( $\beta$ ) <sup>[22]</sup> , 2.04 ( $\epsilon$ ) <sup>[22,31]</sup> , 2.035 (average $\rho$ , 99.5% TMD) <sup>[23]</sup> , 1.985 <sup>[25]</sup> , 2.044 (theoretical $\rho$ ) <sup>[46]</sup> , 1.980 ± 1% (He pycnometry) <sup>[49]</sup> , 2.0355 (3% impurities, sample = crash precipitate from EtOAc/heptane, air pycnometry) <sup>[56]</sup> , 2.0226 (4% impurities, sample = crash precipitate from EtOAc/isopropanol, air pycnometry) <sup>[56]</sup> , 2.0280 (2.4% impurities, sample = crash precipitate from EtOAc/heptane, air pycnometry) <sup>[56]</sup> , 2.0359 (0.5% impurities, sample = crash precipitate from EtOAc/heptane, air pycnometry) <sup>[56]</sup> , 2.0191 (5% impurities, sample = reversible gel recryst. from acrylate gel/EtOAc/CH <sub>2</sub> Cl <sub>2</sub> , air pycnometry) <sup>[56]</sup> , 2.0394 (3% impurities, sample = proprietary from alpha hydrate, single solvent, air pycnometry) <sup>[56]</sup> , 2.0430 (1% impurities, sample = proprietary (evaporative) from solvent/nonsolvent, air pycnometry) <sup>[56]</sup> , 2.0356 (0.5% impurities, sample = crash precipitate from EtOAc/heptane, air pycnometry) <sup>[56]</sup> , 2.0310 (1% impurities, sample = crash precipitate from EtOAc/heptane, air pycnometry) <sup>[56]</sup> , 2.0364 (1% impurities, proprietary sample, single solvent, air pycnometry) <sup>[56]</sup> , 2.04 (@ 298.15 K) <sup>[65]</sup> , 2.001 ( $\alpha$ -, hemihydrate, crystals) <sup>[80]</sup> , 1.981 ( $\alpha$ -form with 0.25 water) <sup>[80]</sup> , 1.985 ( $\beta$ -, anhydrous, recryst. from benzene) <sup>[80]</sup> , 1.916 ( $\gamma$ @ 20 °C) <sup>[80]</sup> , 2.044 ( $\epsilon$ ) <sup>[80]</sup> , 1.98 (X-ray) <sup>[80]</sup> , 1.98 ( $\beta$ -, recryst. from benzene, needle-shaped, prism crystals) <sup>[80]</sup> , densities increase in order: $\gamma$ -, $\alpha$ -, $\beta$ -, $\epsilon$ . <sup>[80]</sup> , 2.035 ( $\epsilon$ -, crystallized using solvent/antisolvent method, use of seed crystals possible) <sup>[86]</sup>		
Heat of formation	98.0 kcal/mol <sup>[38]</sup> , 415 kJ/mol <sup>[31]</sup> , 431.0 ± 13 × 10 <sup>3</sup> J/mol ( $\beta$ -CL-20, $\Delta_fH$ ) <sup>[27,65]</sup> , 377.4 ± 13 × 10 <sup>3</sup> ( $\epsilon$ -CL-20, $\Delta_fH$ ) <sup>[27,65]</sup> , 415.6 kJ/mol ( $\Delta_fH$ ) <sup>[25]</sup> , 103.0 kcal/mol ( $\Delta_fH$ (s)) <sup>[25]</sup> , 921 kJ/kg ( $\Delta_fH$ , ICT thermochemical database) <sup>[33]</sup> , 89.6 kcal/mol ( $\Delta_fH^\circ$ ) <sup>[21]</sup> , 339 kJ/mol ( $\alpha$ -CL-20, enthalpy of form.) <sup>[22]</sup> , 372 kJ/mol ( $\epsilon$ -CL-20, enthalpy of form.) <sup>[22]</sup> , 422.8 kJ/mol (enthalpy of form.) <sup>[35]</sup> , 90.2 kcal mol <sup>-1</sup> ( $\epsilon$ -CL-20, $\Delta_fH^\circ$ ) <sup>[44]</sup> , 96.4 kcal mol <sup>-1</sup> ( $\epsilon$ -CL-20, $\Delta_fH^\circ$ , Finck) <sup>[44]</sup> , 91.1 kcal/mol ( $\epsilon$ -CL-20, $\Delta_fH^\circ$ , Delpeyroux) <sup>[44]</sup> , 90.2 kcal/mol ( $\epsilon$ -CL-20, $\Delta_fH^\circ$ , Simpson) <sup>[44]</sup> , 88.9 kcal/mol ( $\epsilon$ -CL-20, $\Delta_fH^\circ$ , Golfier) <sup>[44]</sup> , 141.0 kcal/mol (enthalpy of form. (g)) <sup>[65]</sup>		
Heat of combustion	-3.649 × 10 <sup>6</sup> J/mol ( $\Delta H_{\text{comb}}$ , $\beta$ -CL-20, exptl., Parr isothermally jacketed calorimeter) <sup>[27,65]</sup> , -3.596 × 10 <sup>6</sup> J/mol ( $\Delta H_{\text{comb}}$ , $\epsilon$ -CL-20, exptl. Parr isothermally jacketed calorimeter) <sup>[27,65]</sup> , $\Delta H_c^\circ$ = -859.97 kcal/mol ( $\epsilon$ -CL-20) <sup>[44]</sup> , $\Delta H_c^\circ$ = -860.3 kcal/mol ( $\epsilon$ -CL-20) <sup>[44]</sup> , $\Delta H_c^\circ$ = -859.4 kcal/mol ( $\epsilon$ -CL-20) <sup>[44]</sup> , $\Delta H_c^\circ$ = -858.1 kcal/mol ( $\epsilon$ -CL-20) <sup>[44]</sup>		
	Calcd. (EXPLO 5.03)	Lit. values	Exptl.
- $\Delta_{\text{ex}}U^\circ$ [kJ kg <sup>-1</sup> ]	6160	6,556 (calcd., K-I) <sup>[10]</sup> 5,966 (calcd., K-W) <sup>[10]</sup> 5.966 (calcd., mod. K-W) <sup>[10]</sup>	6,234 ± 63 (@ 1.96 g cm <sup>-3</sup> , @ 25 °C, $\epsilon$ -CL-20) [H <sub>2</sub> O (l)] <sup>[65]</sup>

		<p>6,168<sup>[4]</sup></p> <p>1.60 kcal/g (<math>Q_{\max}</math>, calcd.)<sup>[25]</sup></p> <p>6,312 (calcd., ICT-code)<sup>[33]</sup></p> <p>6,230<sup>[35]</sup></p> <p><math>6,029 \pm 146</math> (@ 1.96 g cm<sup>-3</sup>, @ 25 °C, ε-CL-20, calcd.) [H<sub>2</sub>O (l)]<sup>[65]</sup></p>	
$T_{ex}$ [K]	4,071	<p>4,095 (@ 2.044 g cm<sup>-3</sup>, calcd.)<sup>[21]</sup></p> <p>4,347 (calcd., ICT code)<sup>[33]</sup></p> <p>3,823 (@ 100% TMD, calcd., Cheetah-6)<sup>[55]</sup></p> <p>4,035 (@ 2.044 g cm<sup>-3</sup>, <math>\Delta H_f = 376.6</math> kJ/mol, calcd., JAGUAR)<sup>[69]</sup></p>	
$p_{C_J}$ [kbar]	445	<p>441 (calcd., K-J)<sup>[10]</sup></p> <p>453 (calcd., K-W)<sup>[10]</sup></p> <p>453 (calcd., mod. K-W)<sup>[10]</sup></p> <p>444<sup>[4]</sup></p> <p>460.6 (@ 2.044 g cm<sup>-3</sup>, calcd.)<sup>[21]</sup></p> <p>422 (@ 1.985 g cm<sup>-3</sup>, calcd.)<sup>[25]</sup></p> <p>147.9 MPa (calcd., ICT-code)<sup>[33]</sup></p>	42.7 GPa (@ 2.04 g cm <sup>-3</sup> ) <sup>[18]</sup>

		468 (@ 100% TMD, calcd., Cheetah-6) <sup>[55]</sup>  45.6 GPa (@ 2.044 g cm <sup>-3</sup> , $\Delta H_f = 376.6 \text{ kJ/mol}$ , calcd., JAGUAR) <sup>[69]</sup>	
VoD [m s <sup>-1</sup> ]	9,778 (@ TMD)	9,620 (@ 2.04 g cm <sup>-3</sup> , calcd., K-J) <sup>[10]</sup>  9,750 (@ 2.04 g cm <sup>-3</sup> , calcd., K-W) <sup>[10]</sup>  9,750 (@ 2.04 g cm <sup>-3</sup> , calcd., mod. K-W) <sup>[10]</sup>  9,380 (@ 2.04 g cm <sup>-3</sup> ) <sup>[4]</sup>  9,833 (@ TMD, calcd., CHEETAH v 8.0) <sup>[12]</sup>  9,480 (@ 1.985 g cm <sup>-3</sup> , calcd.) <sup>[25]</sup>  9,910 (@ 2.044 g cm <sup>-3</sup> , calcd.) <sup>[21]</sup>  9,380 (@ 1.92 g cm <sup>-3</sup> , γ-CL-20) <sup>[65]</sup>  9,380 (@ 1.97 g cm <sup>-3</sup> , α-CL-20) <sup>[65]</sup>  9,380 (@ 1.99 g cm <sup>-3</sup> , β-CL-20) <sup>[65]</sup>  9,660 (@ 2.04 g cm <sup>-3</sup> , ε-CL-20) <sup>[65]</sup>  9,790 (@ 2.044 g cm <sup>-3</sup> , $\Delta H_f = 376.6 \text{ kJ/mol}$ , calcd., JAGUAR) <sup>[69]</sup>	9,570 (@ TMD) <sup>[12]</sup>  9,560 (est. LASEM method) <sup>[12]</sup>  8,470 (@ 1.71 g cm <sup>-3</sup> ) <sup>[18]</sup>  9,400 (@ 2.00 g cm <sup>-3</sup> ) <sup>[18]</sup>  9,460 (@ 2.04 g cm <sup>-3</sup> ) <sup>[18]</sup>  9,800 (@ 2.044 g cm <sup>-3</sup> , extrapolated from data on monocrystal density) <sup>[21]</sup>
$V_0$ [L kg <sup>-1</sup> ]	720		

Exptl. determined detonation calorimetry results (25 g sample, cylinder sample, 1.2 cm diameter, detonated in isothermal calorimetry bomb under 65 Pa vacuum,  $\epsilon$ -CL-20 was detonated within a 1.27 cm annulus of Au for inertial confinement)<sup>[27]</sup>:

Material	$\rho$ (g/cm <sup>3</sup> )	J/g (25 °C, H <sub>2</sub> O (l))	J/cm <sup>3</sup>	J/cm <sup>3</sup> @ TMD
$\epsilon$ -CL-20 (exptl. values)	1.96	6,234 ± 63	12,219 ± 123	12,717 ± 129
$\epsilon$ -CL-20 (calcd. from products)	1.96	6,029 ± 146	11,817 ± 286	12,301 ± 298

Critical diameter [cm]	Critical detonation diameter $d_{c0}$ [mm] and specific surface area, $S_g$ [cm <sup>2</sup> g <sup>-1</sup> ] <sup>[35]</sup> :												
	$S_g$ (cm <sup>2</sup> g <sup>-1</sup> )	$d_{c0}$ (mm)	$S_g$ (cm <sup>2</sup> g <sup>-1</sup> )	$d_{c0}$ (mm)									
	400	2.10	1,550	1.20									
	1,000	1.60	8,000	0.45									
	$d_{c0}$ (mm) @ mean crystal size (μm) <sup>[35]</sup> : 0.45 @ 3 <sup>[35]</sup> , 0.75 @ 10, 1.05 @ 20 <sup>[35]</sup>												
Critical parameters of explosion initiation by impact	critical pressure of explosion initiation, $p_{cr} = 0.43 \pm 0.01$ GPa <sup>[42]</sup> , $\sigma_{ult} = 151$ MPa <sup>[42]</sup>												
Critical initiation $T$ ( $T_b$ ) [°C]	Critical initiation temperature = $T_b$ , $T_{p0}$ = onset $T$ <sup>[64]</sup> :												
	<table border="1"> <thead> <tr> <th>Sample</th> <th><math>T_{p0}</math> (°C)</th> <th><math>T_b</math> (°C)</th> </tr> </thead> <tbody> <tr> <td>Raw CL-20 (Average particle size (<math>d_{50}</math>) = 15.96 μm)</td> <td>223.46</td> <td>232.50</td> </tr> <tr> <td>Nano-CL-20 (Produced by ball milling, average particle size (<math>d_{50}</math>) = 200 nm)</td> <td>215.18</td> <td>224.53</td> </tr> </tbody> </table>				Sample	$T_{p0}$ (°C)	$T_b$ (°C)	Raw CL-20 (Average particle size ( $d_{50}$ ) = 15.96 μm)	223.46	232.50	Nano-CL-20 (Produced by ball milling, average particle size ( $d_{50}$ ) = 200 nm)	215.18	224.53
Sample	$T_{p0}$ (°C)	$T_b$ (°C)											
Raw CL-20 (Average particle size ( $d_{50}$ ) = 15.96 μm)	223.46	232.50											
Nano-CL-20 (Produced by ball milling, average particle size ( $d_{50}$ ) = 200 nm)	215.18	224.53											
Critical $T$ [K]	1058 <sup>[65]</sup> , 1058.0 (est., Joback–Stein method) <sup>[74]</sup> , 1539.4 (Valderrama–Alveraz method) <sup>[74]</sup>												
Critical pressure [bar]	48.9 <sup>[65]</sup> , 48.90 (est., Joback–Stein method) <sup>[74]</sup> , 21.96 (Valderrama–Alveraz method) <sup>[74]</sup>												
SSGT [cm]	Shock sensitivities of micro- and nanosized CL-20 samples (donor charge = RDX refined by acetone with $\rho = 1.48$ g cm <sup>-3</sup> , gap material = polymethyl methacrylate polymer, acceptor charges $\rho = 1.80$ g cm <sup>-3</sup> , inside diameter of charge = 5.10 mm, length of charge = 5.45 mm, $\delta$ = gap thickness, micron-sized CL-20 has, $d_{50} = 40$ –60 μm) <sup>[73]</sup> :												

	Sample	$\delta$ (mm)	$S_{dev}$	
Micron-sized CL-20	43.72	0.42		
Nanosized CL-20	18.31	0.35		
5 s explosion $T$ [°C]	226 ( $\alpha$ -HNIW) <sup>[47]</sup> , 230 ( $\epsilon$ -HNIW) <sup>[47]</sup> , 204 ( $\epsilon$ -HNIW, isothermal conditions with ignition delay of 6.5 min, 10 mg sample) <sup>[47]</sup>			
Ignition $T$ [°C]				
Deflagration point [°C]	220–225 <sup>[65]</sup>			
Vacuum stability test [cm <sup>3</sup> /h]	0.02 cm <sup>3</sup> @ 110 °C/20 h, $\rho_{\epsilon\text{-HNIW}} = 2.02 \text{ g cm}^{-3}$ <sup>[24]</sup> , 0.0 mL/g <sup>[37]</sup> , 1.58 mL and 1.52 mL (1.0 g sample, 40 h @ 100 °C, values recalculated for 2.5 g sample) <sup>[41]</sup> , 0.02 cm <sup>3</sup> @ 110 °C/20 h, $\rho_{\epsilon\text{-HNIW}} = 2.04 \text{ g cm}^{-3}$ <sup>[50]</sup> , 0.4 cm <sup>3</sup> /g @ 100 °C, 193 h <sup>[65]</sup>			
Thermal stability	Isothermal TGA experiments; conversion times for 5% mass loss during isothermal storage of ε-CL20 @ different temperatures <sup>[31]</sup> :			
	$T$ (°C)	5% mass loss conversion time (min)	$T$ (°C)	5% mass loss conversion time (min)
	160	1,141.9	175	215.4
	165	697.8	180	99.6
	170	360.7		
	Thermal stability of polymorphs: $\epsilon$ -> $\gamma$ -> $\alpha$ - <sup>[47]</sup> , ~80% mass loss in air @ 183–211 °C within 200 min <sup>[65]</sup> , thermal stability of polymorphs: $\epsilon$ -> $\gamma$ -> $\alpha$ -hemihydrate > $\beta$ - <sup>[75]</sup>			
	Thermal stability order: $\epsilon$ -> $\gamma$ -> $\alpha$ -hydrate > $\beta$ - (based on DSC, DTA, TGA) <sup>[80]</sup> , thermal stability order: $\alpha$ -hydrate > $\epsilon$ -> $\alpha$ - anhydrous > $\beta$ -> $\gamma$ - (based on phase diagram and pressure studies) <sup>[80]</sup> , heating $\alpha$ -crystals for 2 h in xylenes @ ~130 °C caused discoloration of solvent (becomes yellow) due to HNIW dec. <sup>[83]</sup> , heating $\alpha$ -crystals for 15 min in xylenes @ ~170 °C caused brown discoloration of crystal surfaces <sup>[83]</sup> , accelerated dec. of HNIW in xylenes occurs @ $T$ >130 °C, but pure $\gamma$ -phase crystals grown from $\alpha$ - in xylenes @ 130 °C for 15 min <sup>[83]</sup> , all CL-20 modifications decompose with self-acceleration <sup>[83]</sup> , CL-20 thermal stability: $\epsilon$ -> $\gamma$ -> $\alpha$ - <sup>[83]</sup>			

Approx. mass loss (%) for  $\epsilon$ -CL-20 @ different  $T$ <sup>[83]</sup>:

Time (min)	$T$ (°C)						
	183	187	192	196	202	206	211
20	0	0	0	0	0	2	5
40	0	0	0	2	10	10	32
60	0	0	5	10	25	50	75
80	1	4	10	25	50	70	80
100	2	6	24	45	65	75	80
120	3	9	32	52	70	78	80
140	5	20	50	62	75	80	80
160	6	30	60	70	78	80	80
180	9	43	65	72	80	80	80
200	10	52	70	75	80	—	—
220	18	60	72	78	80	—	—
240	24	62	80	80	80	—	—
260	32	67	80	80	—	—	—
280	40	70	80	80	—	—	—
300	48	71	80	—	—	—	—

Approx. values of mass loss during thermal dec. of CL-20 @ 194 °C:

Time (min)	$\alpha$ -	$\epsilon$ -	$\gamma$ - ( $\alpha$ -)	$\gamma$ - ( $\epsilon$ -)
50	10	1	10	4
100	50	13	53	20
150	72	30	75	40
200	80	45	81	55
225	80	53	81	65

Visual observation on hot-stage microscope: nonsolvated  $\alpha$ -sample crumbled in the  $T$  range of the first endo response (~160 °C); crystals embedded in silicone putty gave vigorous bubbling during fragmentation and conversion. Bubbling not observed during polymorphic conversion of  $\epsilon$ - or  $\beta$ -phases and is consistent with H<sub>2</sub>O loss from the cavities; no high  $T$   $\delta$ -phase was observed for these crystals; heating the sample (@ 10 °C/min) to 200 °C in poly(caprolactone)-triol caused further vigorous bubbling followed by solvation and dec. (blackening of the soln.)<sup>[84]</sup>, dry  $\beta$ - shows very broad transition  $T$  range (~135–226 °C) and the  $\beta$ -crystals observed to phase transition under crossed polarizers; @ ~220–226 °C these same crystals cracked and evolved gas but did not blacken; isothermal heating @ 230 °C caused the crystals to slowly blacken<sup>[84]</sup>, mixture of H<sub>2</sub>O-wetted  $\alpha$ /β-crystals in silicone putty (@ 2 °C/min) gave a superposition of behaviors observed in the two polymorphs<sup>[84]</sup>,  $\beta$ -contaminated  $\gamma$ -samples heated @ 10 °C/min

	showed gas bubbles @ 220 °C with microcracking of the crystals, but no blackening <sup>[84]</sup> , ε-crystals observed to convert under crossed polarizers (@ 10 °C/min) in the endotherm range ~157–176 °C and gas again evolved @ ~220 °C <sup>[84]</sup> , dry ε- crystals left on hot stage for 6 weeks @ 74 °C showed no conversion (FTIR), no fragmentation occurred and no transformation to γ-phase occurred <sup>[84]</sup>																																																								
Vapor pressure [atm. @ °C]	Exptl. determined values: $7.067 \times 10^{-7}$ Pa @ 383.15 K <sup>[65]</sup> , $1.219 \times 10^{-6}$ Pa @ 393.15 K <sup>[65]</sup> , $1.528 \times 10^{-6}$ Pa @ 395.15 K <sup>[65]</sup> , $2.435 \times 10^{-6}$ Pa @ 405.15 K <sup>[65]</sup> , $2.659 \times 10^{-6}$ Pa @ 405.15 K <sup>[65]</sup>																																																								
Burn rate [mm/s]	Burn rate characteristics <sup>[39]</sup> : pressure interval = 0.69–10.3 MPa, pressure exponent = 0.745, burning rate @ 10 MPa = 30.1 mm/s, strand $\rho = 1.96 \text{ g cm}^{-3}$ , adiabatic flame $T$ @ 10 MPa = 3,636 K <sup>[39]</sup>  Pressure interval = 0.1–1.5 MPa, pressure exponent = 0.680, pressure interval = 1.5–20, pressure exponent = 0.775, burning rate @ 10 MPa = 30.1 mm/s, $\rho = 1.96 \text{ g cm}^{-3}$ , adiabatic flame $T$ @ 10 MPa = 3,636 K <sup>[60]</sup>																																																								
Solubility [g/mL]	Almost insoluble in H <sub>2</sub> O (ε-CL-20) <sup>[32]</sup> , good solubility in acetone (ε-CL-20) <sup>[32]</sup> , 3.7 mg/L in H <sub>2</sub> O @ 25 °C <sup>[68]</sup>  CL-20 solubility in plasticizers @ 30 °C <sup>[43]</sup> :  <table border="1"> <thead> <tr> <th>Plasticizer</th> <th>Solubility (g/100 g solvent)</th> <th>Plasticizer</th> <th>Solubility (g/100 g solvent)</th> </tr> </thead> <tbody> <tr> <td>MEN42 (methyl/ethyl nitroso ethyl nitramine)</td> <td>15.8</td> <td>MTN</td> <td>1.1</td> </tr> <tr> <td>DBP (dibutyl phthalate)</td> <td>4.9</td> <td>BDNPA/F</td> <td>1.0</td> </tr> <tr> <td>DOP (dioctyl phthalate)</td> <td>4.5</td> <td>KLO (trinitro/dinitro ethyl benzene)</td> <td>0.7</td> </tr> <tr> <td>BuNENA</td> <td>3.5</td> <td>PolyGLYN</td> <td>0.12</td> </tr> <tr> <td>DOS (dioctyl sebacate)</td> <td>2.8</td> <td>HTPB &lt; 0.1</td> <td></td> </tr> <tr> <td>BTTN</td> <td>1.5</td> <td>PolyNIMMO</td> <td>&lt;0.1</td> </tr> </tbody> </table> $3.86 \times 10^{-3}$ g/L in H <sub>2</sub> O <sup>[65]</sup> , $2.91 \times 10^{-3}$ g/L in H <sub>2</sub> O @ 298.15 K <sup>[65]</sup>  Solubility in H <sub>2</sub> O as function of $T$ (Karakaya) <sup>[65]</sup> :  <table border="1"> <thead> <tr> <th><math>T</math> (°C)</th> <th>mg/L</th> <th><math>T</math> (°C)</th> <th>mg/L</th> </tr> </thead> <tbody> <tr> <td>4</td> <td><math>2.27 \pm 0.09</math></td> <td>45</td> <td><math>11.30 \pm 0.25</math></td> </tr> <tr> <td>19.5</td> <td><math>3.11 \pm 0.06</math></td> <td>50</td> <td><math>14.16 \pm 0.47</math></td> </tr> <tr> <td>25</td> <td><math>4.33 \pm 0.04</math></td> <td>55</td> <td><math>17.37 \pm 0.17</math></td> </tr> <tr> <td>30</td> <td><math>5.46 \pm 0.02</math></td> <td>60</td> <td><math>23.98 \pm 0.41</math></td> </tr> <tr> <td>35</td> <td><math>6.69 \pm 0.01</math></td> <td>65</td> <td><math>32.36 \pm 1.03</math></td> </tr> <tr> <td>39</td> <td><math>8.10 \pm 0.06</math></td> <td>69</td> <td><math>39.68 \pm 0.25</math></td> </tr> </tbody> </table>	Plasticizer	Solubility (g/100 g solvent)	Plasticizer	Solubility (g/100 g solvent)	MEN42 (methyl/ethyl nitroso ethyl nitramine)	15.8	MTN	1.1	DBP (dibutyl phthalate)	4.9	BDNPA/F	1.0	DOP (dioctyl phthalate)	4.5	KLO (trinitro/dinitro ethyl benzene)	0.7	BuNENA	3.5	PolyGLYN	0.12	DOS (dioctyl sebacate)	2.8	HTPB < 0.1		BTTN	1.5	PolyNIMMO	<0.1	$T$ (°C)	mg/L	$T$ (°C)	mg/L	4	$2.27 \pm 0.09$	45	$11.30 \pm 0.25$	19.5	$3.11 \pm 0.06$	50	$14.16 \pm 0.47$	25	$4.33 \pm 0.04$	55	$17.37 \pm 0.17$	30	$5.46 \pm 0.02$	60	$23.98 \pm 0.41$	35	$6.69 \pm 0.01$	65	$32.36 \pm 1.03$	39	$8.10 \pm 0.06$	69	$39.68 \pm 0.25$
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	<p>Aqueous solubility (mg/L) of CL-20 (<i>Monteil-Rivera</i>)<sup>[65]</sup>: 1.95 @ 5 °C, 2.12 @ 10 °C, 2.48 @ 15 °C, 3.16 @ 20 °C, 4.89 @ 30 °C, 7.39 @ 40 °C, 11.62 @ 50 °C, 18.48 @ 60 °C<sup>[65]</sup></p> <p>Solubility in H<sub>2</sub>O @ different <i>T</i> (°C)<sup>[65]</sup>: 3 mg/L @ 4 °C, 2 mg/L @ 5 °C, 2 mg/L @ 11 °C, 3 mg/L @ 16 °C, 3.5 mg/L @ 21 °C, 4 mg/L @ 26 °C, 5 mg/L @ 31 °C, 8 mg/L @ 37 °C, 8 mg/L @ 41 °C, 12 mg/L @ 47 °C, 14 mg/L @ 52 °C, 18 mg/L @ 57 °C, 24 mg/L @ 64 °C, 33 mg/L @ 68 °C, 40 mg/L @ 73 °C<sup>[65]</sup></p> <p><math>3.86 \times 10^{-3}</math> g/L in H<sub>2</sub>O @ 298.15 K (est., <i>Klopman</i>)<sup>[74]</sup>, <math>2.91 \times 10^{-3}</math> g/L in H<sub>2</sub>O @ 298.15 K (est., COSMOtherm)<sup>[74]</sup>, <math>3.65 \times 10^{-3}</math> g/L in H<sub>2</sub>O @ 298.15 K<sup>[74]</sup>, HNIW forms complexes with certain solvents<sup>[80]</sup></p> <p>Solvents with carbonyl groups show high solubility toward HNIW<sup>[82]</sup>, relatively low solubility in FEFO<sup>[83]</sup>, solubility in acetone and ethyl acetate is independent of temperature<sup>[85]</sup></p>																																																															
Hygroscopicity	<p>@ 28 °C, rel. humidity = 90%<sup>[87]</sup>:</p> <table border="1"> <thead> <tr> <th rowspan="2">CL-20</th><th colspan="7">% 1 day    2 days    3 days    4 days    5 days    6 days    12 days</th></tr> <tr> <th>1 day</th><th>2 days</th><th>3 days</th><th>4 days</th><th>5 days</th><th>6 days</th><th>12 days</th></tr> </thead> <tbody> <tr> <td><math>\alpha</math></td><td>0.321</td><td>0.379</td><td>0.422</td><td>0.470</td><td>0.492</td><td>0.519</td><td>0.592</td></tr> <tr> <td><math>\beta</math></td><td>0.013</td><td>0.015</td><td>0.016</td><td>—</td><td>—</td><td>—</td><td>—</td></tr> <tr> <td><math>\gamma</math></td><td>0.014</td><td>0.021</td><td>0.023</td><td>0.025</td><td>—</td><td>—</td><td>—</td></tr> <tr> <td><math>\varepsilon_1</math></td><td>0.006</td><td>0.010</td><td>0.014</td><td>0.019</td><td>0.019</td><td>—</td><td>—</td></tr> <tr> <td><math>\varepsilon_2</math></td><td>0.011</td><td>0.010</td><td>0.014</td><td>0.014</td><td>—</td><td>—</td><td>—</td></tr> <tr> <td><math>\varepsilon_3</math></td><td>0.009</td><td>0.013</td><td>0.013</td><td>—</td><td>—</td><td>—</td><td>—</td></tr> </tbody> </table>	CL-20	% 1 day    2 days    3 days    4 days    5 days    6 days    12 days							1 day	2 days	3 days	4 days	5 days	6 days	12 days	$\alpha$	0.321	0.379	0.422	0.470	0.492	0.519	0.592	$\beta$	0.013	0.015	0.016	—	—	—	—	$\gamma$	0.014	0.021	0.023	0.025	—	—	—	$\varepsilon_1$	0.006	0.010	0.014	0.019	0.019	—	—	$\varepsilon_2$	0.011	0.010	0.014	0.014	—	—	—	$\varepsilon_3$	0.009	0.013	0.013	—	—	—	—
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Compatibility	0.25 cm <sup>3</sup> /g gas evolved (VST @ 110 °C, 20 h, HNIW/TNAZ (60/40), $\rho = 1.92$ g cm <sup>-3</sup> , 98.2% TMD) <sup>[50]</sup>																																																															
Specific heat, $C_p$ [J kg <sup>-1</sup> K <sup>-1</sup> ]	$1004 \pm 13$ <sup>[49]</sup>																																																															
Thermal diffusivity, $D_{th}$ [m <sup>2</sup> s <sup>-1</sup> ]	$0.457 \times 10^{-7} \pm 6\%$ <sup>[49]</sup>																																																															
Thermal conductivity, $\lambda$ [J m <sup>-1</sup> K <sup>-1</sup> s <sup>-1</sup> ]	0.068 <sup>[49]</sup>																																																															
$\Delta H_{dec}$ [J/g]	3,000 (DSC, drilled Al crucible @ 5 K/min) <sup>[49]</sup> , 820.3 (raw $\epsilon$ -HNIW, DSC, floating N <sub>2</sub> atmosphere, @ 10 °C/min) <sup>[61]</sup> , 1,169 (nano- $\epsilon$ -HNIW, DSC, floating N <sub>2</sub> atmosphere, @ 10 °C/min) <sup>[61]</sup> , heat of dec. = 2300 <sup>[65]</sup>																																																															
Activation energy to thermal dec., $E_a$ [kJ/mol]	226.2 (raw $\epsilon$ -HNIW, DSC, floating N <sub>2</sub> atmosphere, @ 10 °C/min) <sup>[61]</sup> , 221.2 (nano- $\epsilon$ -HNIW, DSC, floating N <sub>2</sub> atmosphere, @ 10 °C/min) <sup>[61]</sup> , 151.7 @ 458 477 K (TG) <sup>[65]</sup>																																																															

Dipole moment [D]	1.016 <sup>[65]</sup>
Enthalpy of fusion [kJ/mol]	13.7 <sup>[65,74]</sup> , 42.7 <sup>[65,74]</sup>
Enthalpy of sublimation [kJ/mol]	150–170 <sup>[65]</sup>
Enthalpy of vaporization [kJ/mol]	311 <sup>[65]</sup>
Log $K_{ow}$	1.92 <sup>[65,68]</sup> , 1.375 (predicted value) <sup>[65]</sup> , 4.14 (predicted value) <sup>[65]</sup> , 1.92 (@ 21 °C) <sup>[74]</sup> , 1.38 (est., Ghose method @ 298.15 K) <sup>[74]</sup> , 4.14 (est., COSMOtherm @ 298.15 K) <sup>[74]</sup>
Biodegradation	CL-20 in microcosms to determine biodegradability: CL-20 disappeared in all microcosms after incubation in variety of different soils, CL-20 most rapidly degraded in garden soil, 80% of initial CL-20 disappeared after 2 days of incubation ( <i>Trott</i> ) <sup>[65]</sup> , half life of CL-20 is dependent on the soil type ( <i>Jenkins</i> ) <sup>[65]</sup> : half life = 69 days in Fort Greely soil (est.), 267 days in camp Guernsey soil (est.) and 144 days in Yakima Training Center soil (est.), <i>Phanerochaete chrysosporium</i> and <i>Irpea lacteus</i> bacteria degrade CL-20 with almost all CL-20 removed after 25 days of incubation (also no CL-20 intermediates present) <sup>[65]</sup>
CRT [cm <sup>3</sup> /g]	@ 120 °C for 22 h, 1 atm. He: 0.24 (β-CL-20 LANL sample) <sup>[65]</sup> , 0.16 (ε-, Aerojet sample) <sup>[65]</sup> , 0.10 (ε-, Thiokol sample) <sup>[65]</sup>

	$\gamma\text{-CL-20}^{[13]}$	$\gamma\text{-CL-20}^{[13]}$	$\gamma\text{-CL-20}^{[13]}$	$\gamma\text{-CL-20}^{[13]}$	$\gamma\text{-CL-20}^{[13]}$	$\gamma\text{-CL-20}^{[13]}$	$\varepsilon\text{-CL-20}^{[13]}$	$\varepsilon\text{-CL-20}^{[13]}$	$\varepsilon\text{-CL-20}^{[13]}$	$\varepsilon\text{-CL-20}^{[13]}$	$\varepsilon\text{-CL-20}^{[13]}$	$\zeta\text{-CL-20}$ (high-pressure form) <sup>[15]</sup>	
Chemical formula	$\text{C}_6\text{H}_6\text{N}_{12}\text{O}_{12}$												
Molecular weight [g mol <sup>-1</sup> ]	438.23	438.23	438.23	438.23	438.23	438.23	438.23	438.23	438.23	438.23	438.23	438.23	438.23
Crystal system	Monoclinic	Monoclinic											
Space group	$P2_1/n$	$P2_1/n$											
$a$ [Å]	13.0342(3)	13.2272(7)	13.11670(3)	13.1156(7)	13.0698(4)	8.8628(11)	8.8408(9)	8.8212(10)	8.8004(10)	8.7910(18)	8.789(1)	12.579(2)	
$b$ [Å]	8.1773(2)	8.1692(5)	8.1676(1)	8.1713(4)	8.1737(3)	12.5928(16)	12.5622(12)	12.5368(14)	12.4992(14)	12.481(3)	12.474(1)	7.719(19)	
$c$ [Å]	14.7465(2)	14.8920(8)	14.8436(1)	14.8059(8)	14.718(5)	13.3947(17)	13.3577(13)	13.3330(15)	13.2985(15)	13.285(3)	13.279(1)	14.1260(15)	
$\alpha$ [°]	90	90	90	90	90	90	90	90	90	90	90	90	90
$\beta$ [°]	108.5660(10)	109.164(1)	109.0001(1)	108.841(1)	108.696(1)	106.920(2)	106.820(2)	106.740(2)	106.622(2)	106.55(3)	106.578(1)	111.218(10)	
$\gamma$ [°]	90	90	90	90	90	90	90	90	90	90	90	90	90
$V$ [Å <sup>3</sup> ]	1,489.95(5)	1,520.0(2)	1,509.34(4)	1,501.75(14)	1,494.78(9)	1430.2(3)	1,420.0(2)	1,412.0(3)	1,401.7(3)	1,397.2(5)	1,395.314(1)	1,279.1(4)	
$Z$	4	4	4	4	4	4	4	4	4	4	4	4	4
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.954	1.915	1.929	1.938	1.947	2.035	2.050	2.061	2.077	2.083	2.08	2.275	
$T$ [K]	100	298	250	200	150	298	250	200	150	100	100	293	

	ε-CL-20 <sup>[53]</sup>	α-CL-20 <sup>-1</sup> / <sub>2</sub> H <sub>2</sub> O <sup>[63,65,66]</sup>	β-CL-20 <sup>[63]</sup>	ε-CL-20 <sup>[63]</sup>	γ-CL-20 <sup>[63]</sup>	ε-CL-20 <sup>[65,66]</sup>	β-CL-20 <sup>[65,66]</sup>	γ-CL-20 <sup>[65,66]</sup>
	Large crystals, 300–500 μm length, two nonequivalent molecules in unit cell	X-ray powder diffraction	X-ray powder diffraction	X-ray powder diffraction	X-ray powder diffraction			
Chemical formula	C <sub>6</sub> H <sub>6</sub> N <sub>12</sub> O <sub>12</sub>		C <sub>6</sub> H <sub>6</sub> N <sub>12</sub> O <sub>12</sub>	C <sub>6</sub> H <sub>6</sub> N <sub>12</sub> O <sub>12</sub>	C <sub>6</sub> H <sub>6</sub> N <sub>12</sub> O <sub>12</sub>	C <sub>6</sub> H <sub>6</sub> N <sub>12</sub> O <sub>12</sub>	C <sub>6</sub> H <sub>6</sub> N <sub>12</sub> O <sub>12</sub>	C <sub>6</sub> H <sub>6</sub> N <sub>12</sub> O <sub>12</sub>
Molecular weight [g mol <sup>-1</sup> ]	438.23		438.23	438.23	438.23	438.23	438.23	438.23
Crystal system	Monoclinic	Orthorhombic	Orthorhombic	Monoclinic	Monoclinic	Orthorhombic	Monoclinic	Monoclinic
Space group	P2 <sub>1</sub>	Pbca	Pb2 <sub>1</sub> a	P2 <sub>1</sub> /n	P2 <sub>1</sub> /n	P2 <sub>1</sub> /a	Pca2 <sub>1</sub>	P2 <sub>1</sub> /n
<i>a</i> [Å]	8.861(3)	9.478	9.676	8.852	13.231	13.748	9.652	13.213
<i>b</i> [Å]	12.608(8)	13.206	13.006	12.556	8.170	12.596	11.644	8.161
<i>c</i> [Å]	13.333(8)	23.561	11.649	13.386	14.876	8.867	13.002	14.898
α [°]	90	90	90	90	90	90	90	90
β [°]	106.89(6)	90	90	106.820	109.170	111.9	90	109.12
γ [°]	90	90	90	90	90	90	90	90
<i>V</i> [Å <sup>3</sup> ]	1,425.41(9)	2,948.92	1,465.98	1,424.15	1,518.89			
<i>Z</i>	4							
<i>ρ</i> <sub>calc</sub> [g cm <sup>-3</sup> ]	2.041(7)							
<i>T</i> [K]	383	30–130 °C	30–120 °C	30–130 °C	30–180 °C	30–180 °C		



$\beta$ [°]	90	90	109.21(9)	106.88(2)	90	90	109.17	106.82
$\gamma$ [°]	90	90	90	90	90	90	90	90
$V$ [Å <sup>3</sup> ]	2,985.2(8)	1,465.7(5)	1,511.3(14)	1,432.0(4)				
$Z$	8	4	4	4				
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.97	1.986	1.926	2.033	1.981	1.985	1.916	2.044
$T$ [K]	293	293	293	293	20 °C	20 °C	20 °C	20 °C

Linear CTEs<sup>[63]</sup>:  $\epsilon$ -CL-20 shows isotropic expansion in  $T$  range 30–130 °C<sup>[63]</sup>,  $\alpha$ -CL-20 shows anisotropic expansion in  $T$  range 30–130 °C<sup>[63]</sup>,  $\beta$ -CL-20 shows anisotropic expansion in  $T$  range 30–120 °C<sup>[63]</sup>,  $\gamma$ -CL-20 shows anisotropic expansion in  $T$  range 30–180 °C.<sup>[63]</sup>

Polymorph	$\alpha_a$ (10 <sup>-5</sup> °C <sup>-1</sup> )	$\alpha_b$ (10 <sup>-5</sup> °C <sup>-1</sup> )	$\alpha_c$ (10 <sup>-5</sup> °C <sup>-1</sup> )	$\alpha_\beta$ (10 <sup>-5</sup> °C <sup>-1</sup> )	$\alpha_{\text{volume}}$ (10 <sup>-5</sup> °C <sup>-1</sup> )	$T$ range (°C)	Ref.
$\alpha$ -CL-20· <sub>1/2</sub> H <sub>2</sub> O	2.22	4.55	7.97		11.02	30–130	[63]
	-7.55						[63]
	3.56	5.04	6.18		14.90	130–30	[63]
Anhydrous $\alpha$ -CL-20	2.80	5.26	7.23		15.39	30–130	[63]
$\beta$ -CL-20	5.35	1.48	6.61		13.52	30–120	[63]
$\epsilon$ -CL-20	4.95	4.91	4.40	1.43	13.50	30–130	[63]
$\gamma$ -CL-20	8.72	-0.75	6.40	3.70	11.90	30–180	[63]
$\beta$ -CL-20	2.56	1.71	1.09		6.41	-169 to 152	[63]
$\epsilon$ -CL-20	1.77	2.26	2.14		5.71	-169 to 152	[63]
$\gamma$ -CL-20	2.70	2.48	2.64		5.85	-169 to 152	[63]

Large crystals of  $\epsilon$ -CL-20 consisting of perfect crystals of 300–500 µm length showed synchronous extinction under polarized light and symmetry  $P2_1$  (rather than the usual  $P2_1/n$ ) with two nonequivalent molecules with slightly different conformations,  $\rho = 2.062 \text{ g cm}^{-3}$ <sup>[53]</sup>

Five different polymorphs of CL-20 have been identified and reported in the literature, namely:  $\alpha$ -,  $\beta$ -,  $\gamma$ -,  $\epsilon$ -, and  $\zeta$ - and four out of these five polymorphs ( $\alpha$ -,  $\beta$ -,  $\gamma$ -,  $\epsilon$ -) exist under ambient temperature and pressure<sup>[46]</sup>

Recrystallization of  $\epsilon$ -polymorph using the concentration process: acetone, esters and aromatic solvents are best to obtain particle size 10–15 µm<sup>[22]</sup>

The recrystallization method of precipitation with an antisolvent has the advantage of occurring at low temperature which allows avoiding the  $\epsilon$ -  $\rightarrow$   $\gamma$ -phase transition<sup>[85]</sup>. The high nucleation rate of this method should favor the formation of the kinetically favored polymorph,  $\beta$ .<sup>[85]</sup>

Inoculation of a saturated CL-20 acetone/toluene (solvent/antisolvent) mixture with a few  $\epsilon$ -CL-20 crystals, followed by reduction in volume of acetone present produces  $\epsilon$ -CL-20 crystals as agglomerates with 100–180 µm diameter (crystal size was dependent on size of inoculation crystals and rate of acetone removal)<sup>[85]</sup>. The technique of solvent evaporation with/without ultrasound was used to produce  $\epsilon$ -CL-20 crystals with bipyramidal or rhombic shapes with no agglomerates; solvent evaporation in combination with in-situ ultrasound resulted in smoothing of the sharp edge of bipyramidal crystals and shows fewer larger-sized particles surrounded by fine-sized particles. The mean particle size was 30–40 µm using the ultrasound technique<sup>[85]</sup>. In evaporative crystallization, the density of the  $\epsilon$ -CL-20 crystals obtained depends on the evaporation rate, CL-20 concentration and temperature<sup>[85]</sup>.

The phase transition from  $\epsilon$ -CL-20 to  $\beta$ -CL-20 occurred when the evaporation rate was increased above 0.125 mL/h @ 70 °C<sup>[85]</sup>. The use of crystal growth modifiers was reported, such as amino acetic acid which resulted in spheroidal-shaped crystals<sup>[85]</sup>. Cuboidal-shaped crystals were obtained using the solvent stripping-off with two crystal growth modifiers approach (1% TPT)<sup>[85]</sup>; the use of solvent/anti-solvent technique to produce  $\epsilon$ -CL-20 with or without the use of seed crystals is given in detail in<sup>[86]</sup>.

The effect of time on CL-20 vacuo evaporative crystallization processes run with an addition of 1% by vol. acetic acid as crystal growth modifier, but no CL-20 seed crystals; crystal appearance = rounded-edged cubes ca. 100  $\mu\text{m}$  size, agglomerate formation unavoidable but reduced in number on longer process times,  $\epsilon$ -polymorph formed (FTIR)<sup>[85]</sup>:

No.	Crystallization time (h)	Crystallization pressure (kPa)	Crystallization yield (%)	Crystallographic purity (%)	Crystal density ( $\text{g cm}^{-3}$ )
1	2	4.67	96	95 ± 1	2.008 ± 0.004
2	3	4.67	96	95 ± 1	2.007 ± 0.004
3	5	4.67	97	94 ± 1	2.002 ± 0.004

The effect of pressure on the CL-20 in vacuo evaporative crystallization processes run with an addition of 1% by vol. 1,2,5-triacetoxypentane as crystal growth modifier, but no CL-20 seed crystals; crystal appearance = cubes and bipyramids, best crystals obtained using 6.67 kPa pressure,  $\epsilon$ -polymorph formed (FTIR)<sup>[85]</sup>:

No.	Crystallization time (h)	Crystallization pressure (kPa)	Crystallization yield (%)	Crystallographic purity (%)	Crystal density ( $\text{g cm}^{-3}$ )
4	3	5.33	95	95 ± 1	2.026 ± 0.003
5	3	6.67	93	95 ± 1	2.021 ± 0.004
6	3	8.00	90	94 ± 1	2.010 ± 0.004

The effect of the crystallization nuclei added on the CL-20 in vacuo evaporative crystallization processes run with an addition of 1% by vol. 1,2,5-triacetoxypentane as crystal growth modifier, crystallization nuclei added, pressure maintained at 6.67 kPa during 4 h process, crystal appearance = cubic shape with rounded edges<sup>[85]</sup>:

No.	Crystallization time (h)	Crystallization pressure (kPa)	Crystallization yield (%)	Crystallographic purity (%)	Crystal density ( $\text{g cm}^{-3}$ )
7	4	—	95	95 ± 1	2.026 ± 0.004
8	4	0.5	93	95 ± 1	2.021 ± 0.004

The effect of a crystal growth modifier on the CL-20 in the vacuo evaporative crystallization processes run with an addition of 1% with respect to CL-20 crystal growth modifier, 6.67 kPa pressure maintained, process temperature = 35 °C and 60 rpm flask rotation speed; crystal shape = similar to spherical with smooth, rounded edges for 1,2,5-triacetoxypentane, glycine or triacetin, cubic and bipyramidal forms if ethylene glycol added with significant quantities of agglomerates formed, bipyramids and cubes of up

to 400 µm with lower quantities of agglomerates if diethylene glycol used; cubic crystals of ca. 200 µm obtained with significant quantities of fine crystals if formic acid, acetone or ethyl alcohol used<sup>[85]</sup>.

No.	Crystal growth modifier	Crystallization yield (%)	Crystallographic purity (%)	Crystal density (g cm <sup>-3</sup> )
9	1,2,5-Triacetoxypentane	95	95 ± 1	2.021 ± 0.004
10	Glycine	95	97 ± 1	2.030 ± 0.004
11	Ethylene glycol	93	97 ± 1	2.029 ± 0.003
12	Diethylene glycol	97	95 ± 1	2.025 ± 0.005
13	Formic acid	90	98 ± 1	2.031 ± 0.005
14	Triacetin	77	95 ± 1	2.026 ± 0.003
15	Ethyl alcohol	79	99 ± 1	2.041 ± 0.007
16	Acetone	94	98 ± 1	2.037 ± 0.006

Crystal modification obtained using the nonsolvent method<sup>[58]</sup>:

HNIW soln.	Nonsolvent	Dipole moment of nonsolvent	HNIW crystal modification
Ethyl acetate	Petroleum ether		ε-
Acetone	Petroleum ether		ε-
Ethyl acetate	Petroleum ether		ε-
Ethyl acetate	Isooctane	0	ε-
Ethyl acetate	Cyclohexane	0	ε-
Acetone	Toluene	0.39	ε-
Ethyl acetate	Trichloromethane	1.55	Mixture of α-, ε-
Acetone	Petroleum ether		ε-
Acetone	Toluene	0	ε-
Acetone	Cyclohexane	0	ε-
Ethyl acetate	Tetrachloromethane	0	ε-
Ethyl acetate	Ethyl alcohol	1.68	Mixture of α-, ε-
Triethylene glycol		5.0	α-

α-CL-20·<sub>1/2</sub> H<sub>2</sub>O prepared by recryst. from acetone<sup>[63]</sup>, β-CL-20 prepared by recryst. from trichloroethane<sup>[63]</sup>, ε-CL-20 prepared by recryst. from ethyl acetate.<sup>[63]</sup>

Cavity occupancy of 17–50% water in α-crystal lattice (X-ray).<sup>[83]</sup>

Round Robin results<sup>[67]</sup>:

Sample source	Precursor used in synth.	Cl-20 used for recryst.	Recryst. method	Particle size distribution of tested sample (micron)	BET surface area (m <sup>2</sup> /g)	IS(Indian Head, ERL app., 50% height, cm) <sup>a</sup>	IS(China Lake, ERL app., 50% height, cm) <sup>b</sup>	IS(TACOM-ARDC, ERL app., 50% height, cm) <sup>d</sup>	IS(Thiokol, ABL app., 50% height, cm) <sup>e</sup>	IS(Thiokol, ABL app., TIL, cm) <sup>f</sup>
		Chemical purity (% Cl-20)	Polymorph purity (% ε-)	10%	50%	90%				
Thiokol	TADF	97	>95	Evap.	70	141	217	0.0367	8	5
Thiokol	TADF	97	>95	Evap.	71	141	221	0.0474	10	9
Thiokol	TADF	96	>95	Crash precip.	85	166	232	0.0759	8	9
Thiokol	TADA	99	>95	Crash precip.	62	159	222	0.0525	10	10
China Lake	TADF	97.5	95	Trisolvent recryst.	15	35	73	0.2108	12	9
China Lake	TADF	95	95	Thermoreversible gel recryst.	51	175	400	0.1823	9	11
China Lake	TADF	96	95	Thermoreversible gel recryst.	100	258	467	0.1075	13	10
Indian Head	TADF	97.6	>95	Crash precip.	30	141	317	0.1175	9	10
Indian Head	TADF	99.5	>95	Crash precip.	23	185	311	0.0745	12	9

Thiokol	TADF	97	>95	Crash precip.	50	157	343	0.0844	10	7	6	13.4	3.5	5.5
Thiokol	TADF	97	>95	Crash precip.	50	157	343	0.0844	10	9	6	—	3.5	4.6
Thiokol	TADF	97	>95	Crash precip.	50	157	343	0.0844	12	21	16	18.2	1.8	5.7
Aerojet	TAIW	>99.9	>90	Proprietary process	—	40	—	0.0764	9	8	6	12.5	3.5	5.0
TACOM-ARDEC	TADF	>97	>97	Proprietary process from $\alpha$ -hydrate	—	12.5-25	—	0.1204	12	15	13	13.8	1.8	4.0
Nexpro-Bofors	—	98.6	—	Proprietary process	93	180	307	0.1101	10	8	8	12.4	3.5	4.3
SNPE	—	99	>95	Proprietary evap. process	12	27	50	0.2765	10	12	10	39.0	1.8	5.0

<sup>a</sup>Indian Head, ERL impact apparatus, type 12 tool, 2.5 kg mass, 35 mg sample, 50% probability of reaction, noise meter;

<sup>b</sup>China Lake, ERL impact apparatus, type 12 tool, 2.5 kg mass, garnet sandpaper, 50% probability of reaction, smudge on sandpaper and smoke, spark, odor or noise observed; <sup>c</sup>China Lake, ERL impact apparatus, type 12 tool, 2.5 kg mass, garnet sandpaper, low-fire point = lowest level at which fire is obtained, approx. the level at which the sample will fire 10% of the time; <sup>d</sup>TACOM-ARDEC, ERL impact apparatus, type 12 tool, 2.5 kg mass, 50% probability of reaction; <sup>e</sup>Thiokol, ABL impact apparatus, 2 kg mass, 50% probability of reaction; <sup>f</sup>Thiokol, ABL impact apparatus, 2 kg mass, TIL = threshold initiation level, corresponds to no “go” in 10 consecutive tests.

Round Robin results<sup>[67]</sup>:

Sample source	Precursor used in synth.	CL-20 used for recryst.	Recryst. method	Particle size distribution of tested sample (micron)		BET surface area (m <sup>2</sup> /g)	FS (Indian Head, ABL app., 50% point @ 8 ft/s) (lb) <sup>b</sup>	FS (China Lake, ABL app., 50% point @ 8 ft/s) (lb) <sup>c</sup>	FS (TACOM-ARDEC, BAM app., TIL, kg) <sup>d</sup>	FS (Thiokol, ABL app., TIL, lb) <sup>e</sup>	FS (Thiokol, ABL app., 50% point @ 8 ft/s) (lb) <sup>f</sup>			
				10%	50%									
			Chemical purity (% CL-20)	Polymorph purity (%) ε-										
Thiokol	TADF	97	>95	Evap.	70	141	217	0.0367	75	155	126	11.2	25 @ 3 ft/s	371
Thiokol	TADF	97	>95	Evap.	71	141	221	0.0474	<30	159	159	12.8	25 @ 32 ft/s	165
Thiokol	TADF	96	>95	Crash precip.	85	166	232	0.0759	30	74	63	12.8	180 @ 2 ft/s	188
Thiokol	TADA	99	>95	Crash precip.	62	159	222	0.0525	<30	85	50	16	25 @ 4 ft/s	205
China Lake	TADF	97.5	95	Trisolvant recryst.	15	35	73	0.2108	<30	170	159	21.6	130 @ 2 ft/s	195
China Lake	TADF	95	95	Thermoreversible gel recryst.	51	175	400	0.1823	55	148	126	19.2	25 @ 4 ft/s	260
China Lake	TADF	96	95	Thermoreversible gel recryst.	100	258	467	0.1075	<30	129	126	25.2	50 @ 4 ft/s	185
Indian Head	TADF	97.6	>95	Crash precip.	30	141	317	0.1175	40	65	50	12.8	50 @ 3 ft/s	170

Indian Head	TADF	99.5	>95	Crash precip.	23	185	311	0.0745	<30	112	63	16.8	50 @ 4 ft/s	210
Thiokol	TADF	97	>95	Crash precip.	50	157	343	0.0844	55	91	63	14.4	50 @ 2 ft/s	252
Thiokol	TADF	97	>95	Crash precip.	50	157	343	0.0844	55	63	98	-	50 @ 6 ft/s	255
Thiokol	TADF	97	>95	Crash precip.	50	157	343	0.0844	<30	141	126	6.4	50 @ 4 ft/s	-
Aerojet	TAIW	>99.9	>90	Proprietary process	-	40	-	0.0764	30	105	79	16	25 @ 4 ft/s	163
TACOM-ARDEC	TADF	>97	>97	Proprietary process from $\alpha$ -hydrate	-	12.5-25	-	0.1204	<30	200	159	12	25 @ 6 ft/s	185
Nexpol-Bofors	-	98.6		Proprietary process	93	180	307	0.1101	<30	200	200	12	25 @ 8 ft/s	195
SNPE	-	99	>95	Proprietary evap. process	12	27	50	0.2765	<30	85	50	9.6	50 @ 8 ft/s	-

<sup>a</sup>Indian Head, ABL sliding friction apparatus, steel wheel, steel plate, standard speed of wheel = 8 ft/s, 35–45 mg sample, values reported as gage pressure readings at ft/sec; <sup>b</sup>China Lake, sliding friction apparatus, same details as above, speed of plate = 8 ft/s, positive test detected by smudge, observation of smoke, spark, odor or fire, results as force at which sample ignites 50% of the time; China Lake, sliding friction apparatus, same details as above, speed of plate = 8 ft/s, positive test detected by smudge, observation of smoke, spark, odor or fire, low-fire point = lowest level at which fire is obtained, approx. the level at which the sample will fire 10% of the time; <sup>d</sup>TACOM-ARDEC, BAM friction apparatus, porcelain plate and porcelain pin, max. value of 360 N, results observed as flash, smoke or noise, TIL = threshold initiation level in which no reaction observed in 10 trials; <sup>e</sup>Thiokol, sliding friction apparatus, as above, TIL = threshold initiation level, corresponds to no "go" in 20 consecutive tests; <sup>f</sup>Thiokol, sliding friction apparatus, as above,  $H_{50\%}$  = 50% ignition level.

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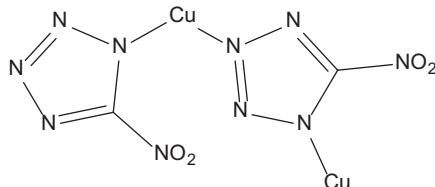
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## Copper(I) 5-nitrotetrazolate

Name [German, acronym]: Copper(I) 5-nitrotetrazolate [kupfer(I)-5-nitrotetrazolat, DBX-1]

Main (potential) use: “Drop-in” replacement for lead azide<sup>[1,10]</sup>

Structural formula:



	<b>DBX-1</b>												
Formula	C <sub>2</sub> Cu <sub>2</sub> N <sub>10</sub> O <sub>4</sub>												
Molecular mass [g mol <sup>-1</sup> ]	355.18												
Appearance at RT	Crystalline red-brown solid <sup>[1]</sup> , brown crystals <sup>[7]</sup> , rust-colored crystals <sup>[8]</sup>												
IS [J]	<p>0.036 ± 0.012<sup>[1,6]</sup>, 0.04 Nm<sup>[2]</sup>, 0.036<sup>[3,4]</sup>, 0.040 ± 0.010 (ball drop)<sup>[11]</sup>,            0.040 ± 0.01 (ball drop, NATO AOP-7)<sup>[7]</sup>, no go @ 30 in (ball drop)<sup>[8]</sup>, no go            @ 8 in (ball drop)<sup>[8]</sup>, no go @ 4 in (ball drop)<sup>[8]</sup>, 0.057 ± 0.006 (ball drop            apparatus)<sup>[9]</sup></p> <p>Ball drop instrument<sup>[11]</sup>:</p> <table border="1"> <thead> <tr> <th>Sample</th><th>Impact (J)</th></tr> </thead> <tbody> <tr> <td>DBX-1, T = 0 month</td><td>0.036 ± 0.012</td></tr> <tr> <td>DBX-1, T = 6 months</td><td>0.042 ± 0.003</td></tr> <tr> <td>DBX-1, T = 12 months</td><td>0.038 ± 0.013</td></tr> <tr> <td>DBX-1, T = 12 months (unaged)</td><td>0.037 ± 0.004</td></tr> <tr> <td>DBX-1, previous contract</td><td>0.040 ± 0.010</td></tr> </tbody> </table>	Sample	Impact (J)	DBX-1, T = 0 month	0.036 ± 0.012	DBX-1, T = 6 months	0.042 ± 0.003	DBX-1, T = 12 months	0.038 ± 0.013	DBX-1, T = 12 months (unaged)	0.037 ± 0.004	DBX-1, previous contract	0.040 ± 0.010
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DBX-1, T = 12 months (unaged)	0.037 ± 0.004												
DBX-1, previous contract	0.040 ± 0.010												
FS [N]	0.098 <sup>[1,6]</sup> , 0.1 <sup>[2,3,5]</sup> , >0.098 <sup>[4]</sup> , no fire = 0 g, low fire = 10 g (small BAM) <sup>[11]</sup> , no fire level = 10 g, fire level = 0 g (Julius-Peters, BAM, max. load of 2,075 g) <sup>[7]</sup> , go @ 0.1 (BAM) <sup>[8]</sup> , no fire = 20 g, low fire = 30 g (BAM) <sup>[9]</sup> , no fire = 0 N, low fire = 0.098 N (Julius-Peters small BAM) <sup>[1]</sup>												

Julius-Peters, small BAM<sup>[11]</sup>:

	Sample	No fire level (g)	Min. fire level (g)
DBX-1, $T = 0$ month	0	10	
DBX-1, $T = 6$ months	0	10	
DBX-1, $T = 12$ months	0	10	
DBX-1, $T = 12$ months (unaged)	0	10	
DBX-1, previous contract	0	10	
ESD [J]	0.000012 <sup>[1,6]</sup> , 3.1 mJ <sup>[3]</sup> , 12 µJ <sup>[4]</sup> , 3.1 mJ <sup>[3,5]</sup> , 12 µJ (LEESA) <sup>[11]</sup> , no go @ 0.0016 (AOP-7) <sup>[8]</sup> , no go @ 0.0025 (AOP-7) <sup>[8]</sup> , no go @ 0.0020 (AOP-7) <sup>[8]</sup> , 12 µJ (minimum fire level, LEESA) <sup>[1]</sup>		
	ESD testing – LEESA <sup>[11]</sup> :		
	Sample	Minimum fire level (µJ)	
DBX-1, $T = 0$ month	12		
DBX-1, $T = 6$ months	12		
DBX-1, $T = 12$ months	12		
DBX-1, $T = 12$ months (unaged)	12		
DBX-1, previous contract	12		
$N$ [%]	39.44		
$\Omega(\text{CO}_2)$ [%]	-9.0 (to Cu <sub>2</sub> O), -18.02% (to CuO) <sup>[11]</sup>		
$T_{\text{dec.}}$ [°C]	337.69 (DSC @ 20 K/min, sealed Al cups) <sup>[1]</sup> , 337 <sup>[4]</sup> , 325 <sup>[5]</sup> , 329 (onset), 337 (peak) (DSC @ 20 °C/min) <sup>[11]</sup> , 260 (onset of weight loss, high res. TGA) <sup>[11]</sup> , 326 (onset), 333 (peak) (DSC) <sup>[11]</sup> , 310 (DSC) <sup>[6]</sup> , 325.2 (DSC, DBX-1 from CuCl <sub>2</sub> and sodium nitrotetrazolate dihydrate, product dried @ 70 °C in oven) <sup>[7]</sup> , 331.7 (DSC, DBX-1 from CuCl <sub>2</sub> and sodium nitrotetrazolate dihydrate, air-dried crystals) <sup>[7]</sup> , 331.8 (DSC, DBX-1 from CuCl <sub>2</sub> and sodium nitrotetrazolate dihydrate, air-dried crystals) <sup>[7]</sup> , 333 (dec. max., DSC) <sup>[3]</sup> , 270 (onset), 283 (peak max.) (DSC @ 20 °C/min) <sup>[9]</sup> , 302.8 (onset, 0.315 mg sample, DSC @ 5 °C/min) <sup>[10]</sup> Aged samples, DSC @ 20 °C/min, exo peak max.: 333.21 (aged 0 months), 333.79 (aged 6 months), 333.79 (after 12 months, unaged), 333.50 (aged 12 months) <sup>[11]</sup>		
$\rho$ [g cm <sup>-3</sup> ]	2.584 (@ 113 K) <sup>[1]</sup> , ~2.58 <sup>[3]</sup> , 2.59 (crystal) <sup>[3]</sup> , 2.07 <sup>[9]</sup> , 4.80 <sup>[6]</sup> , 2.81 ± 0.005 (He pycnometry) <sup>[7]</sup> , 2.58 (X-ray) <sup>[11]</sup> , 2.59 (He pycnometry) <sup>[11]</sup>		
Heat of formation	67.08 cal/g <sup>[11]</sup> , 280.9 J/g (bomb calorimetry) <sup>[1]</sup> , 99.8 kJ/mol (enthalpy of form.) <sup>[2]</sup> , 280.9 kJ/mol ( $\Delta_f H^\circ$ ) <sup>[3,4]</sup>		

	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.																																																																												
$-\Delta_{\text{ex}}U^{\circ} [\text{kJ kg}^{-1}]$		3816.6 <sup>[3]</sup> 911.59 cal/g <sup>[11]</sup>	3,816.6 (bomb calorimetry) <sup>[1,3]</sup>																																																																												
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$p_{\text{C-J}} [\text{GPa}]$																																																																															
VoD [ $\text{m s}^{-1}$ ]			<p>7,000 (@ 2.58 <math>\text{g cm}^{-3}</math>)<sup>[2]</sup></p> <p>DBX-1 @ <math>1.6 \pm 0.1 \text{ g cm}^{-3}</math>, glass capillary for all microcapillaries that detonated<sup>[12]</sup>:</p> <table border="1"> <thead> <tr> <th>Capillary diameter (mm)</th> <th>Detonation velocity (mm/<math>\mu\text{s}</math>)</th> <th>Column mass (mg)</th> <th>Column height (mm)</th> </tr> </thead> <tbody> <tr><td>0.480</td><td><math>3.492 \pm 0.090</math></td><td>1.31</td><td>4.50</td></tr> <tr><td>0.480</td><td><math>4.832 \pm 0.102</math></td><td>1.42</td><td>3.99</td></tr> <tr><td>0.480</td><td><math>4.425 \pm 0.098</math></td><td>1.12</td><td>3.50</td></tr> <tr><td>0.480</td><td><math>4.407 \pm 0.090</math></td><td>2.59</td><td>8.80</td></tr> <tr><td>0.480</td><td><math>4.261 \pm 0.087</math></td><td>3.65</td><td>11.84</td></tr> <tr><td>0.399</td><td><math>4.120 \pm 0.088</math></td><td>1.55</td><td>7.51</td></tr> <tr><td>0.399</td><td><math>4.216 \pm 0.087</math></td><td>1.41</td><td>7.04</td></tr> <tr><td>0.282</td><td><math>3.425 \pm 0.072</math></td><td>0.96</td><td>9.61</td></tr> <tr><td>0.282</td><td><math>3.277 \pm 0.068</math></td><td>0.94</td><td>9.36</td></tr> <tr><td>0.282</td><td><math>3.228 \pm 0.066</math></td><td>0.92</td><td>9.43</td></tr> <tr><td>0.201</td><td><math>3.222 \pm 0.066</math></td><td>0.40</td><td>7.65</td></tr> <tr><td>0.201</td><td><math>3.073 \pm 0.062</math></td><td>0.82</td><td>16.44</td></tr> <tr><td>0.201</td><td><math>3.417 \pm 0.077</math></td><td>0.18</td><td>2.90</td></tr> <tr><td>0.142</td><td><math>3.005 \pm 0.062</math></td><td>0.25</td><td>9.12</td></tr> <tr><td>0.142</td><td><math>2.991 \pm 0.062</math></td><td>0.17</td><td>5.43</td></tr> <tr><td>0.099</td><td><math>2.881 \pm 0.059</math></td><td>0.34</td><td>23.5</td></tr> <tr><td>0.099</td><td><math>2.990 \pm 0.061</math></td><td>0.14</td><td>7.80</td></tr> <tr><td>0.099</td><td><math>2.834 \pm 0.0574</math></td><td>0.24</td><td>17.02</td></tr> </tbody> </table>	Capillary diameter (mm)	Detonation velocity (mm/ $\mu\text{s}$ )	Column mass (mg)	Column height (mm)	0.480	$3.492 \pm 0.090$	1.31	4.50	0.480	$4.832 \pm 0.102$	1.42	3.99	0.480	$4.425 \pm 0.098$	1.12	3.50	0.480	$4.407 \pm 0.090$	2.59	8.80	0.480	$4.261 \pm 0.087$	3.65	11.84	0.399	$4.120 \pm 0.088$	1.55	7.51	0.399	$4.216 \pm 0.087$	1.41	7.04	0.282	$3.425 \pm 0.072$	0.96	9.61	0.282	$3.277 \pm 0.068$	0.94	9.36	0.282	$3.228 \pm 0.066$	0.92	9.43	0.201	$3.222 \pm 0.066$	0.40	7.65	0.201	$3.073 \pm 0.062$	0.82	16.44	0.201	$3.417 \pm 0.077$	0.18	2.90	0.142	$3.005 \pm 0.062$	0.25	9.12	0.142	$2.991 \pm 0.062$	0.17	5.43	0.099	$2.881 \pm 0.059$	0.34	23.5	0.099	$2.990 \pm 0.061$	0.14	7.80	0.099	$2.834 \pm 0.0574$	0.24	17.02
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Critical diameter [cm]	<0.1 mm (DBX-1 @ $1.6 \pm 0.1 \text{ g cm}^{-3}$ (58–66% dense) with glass confinement, DBX-1 milled with isopropyl alcohol to achieve average particle size of 4.65 $\mu\text{m}$ ) <sup>[12]</sup>																					
Critical temperature, $T_c$ [ $^{\circ}\text{C}$ ]	256–281 (0.64 cm diameter cylinder @ 80% TMD) <sup>[1]</sup>																					
Initiating ability	Priming ability test: minimum charge in model detonator toward RDX = 0.025 g <sup>[3]</sup>																					
explosion $T$ [ $^{\circ}\text{C}$ ] 1 s ignition $T$ [ $^{\circ}\text{C}$ ] 5 s ignition $T$ [ $^{\circ}\text{C}$ ] Ignition $T$ [ $^{\circ}\text{C}$ ]	350.7 (5 s, hot-stage apparatus) <sup>[1]</sup> , 356.2 (1 s, hot-stage apparatus) <sup>[1]</sup> , 345.2 (10 s, hot-stage apparatus) <sup>[1]</sup> 356 <sup>[3,11]</sup> 351 <sup>[3,11]</sup> Ignition temperature via hot-stage, data from ref. <sup>[11]</sup> : 356 (1 s) <sup>[11]</sup> , 351 (5 s) <sup>[11]</sup> , 345 (10 s) <sup>[11]</sup>																					
Vacuum stability test [ $\text{cm}^3/\text{h}$ ]	0.470 mL/g (0.025 g, 100 $^{\circ}\text{C}$ , 48 h) <sup>[1,11]</sup>																					
Thermal stability	0% mass loss after 24 h @ 181 $^{\circ}\text{C}$ (convection oven) <sup>[1,3]</sup> , quite stable under air and can be stored for extended periods of time under ambient conditions <sup>[10]</sup> , 260 $^{\circ}\text{C}$ (onset of weight loss, high-res. TGA) <sup>[11]</sup> , 0% weight loss after 24 h @ 181 $^{\circ}\text{C}$ <sup>[11]</sup> , no aging effects after storage @ 70 $^{\circ}\text{C}$ for 6 or 12 months, or for 12 months @ 31% RH @ ambient temperature <sup>[1]</sup>  Aged samples, DSC @ 20 $^{\circ}\text{C}/\text{min}$ , exo peak max.: 333.21 (aged 0 months), 333.79 (aged 6 months), 333.79 (after 12 months, unaged), 333.50 (aged 12 months) <sup>[11]</sup>																					
Hygroscopicity	Nonhygroscopic, gains less than 0.1% surface moisture over time, independent of particle size or humidity <sup>[1]</sup>  Data from ref. <sup>[1,11]</sup> :  <table border="1"> <thead> <tr> <th>Hygroscopicity @ 25 <math>^{\circ}\text{C}</math></th> <th>Large particle (EL3C106A) ~110 <math>\mu\text{m}</math></th> <th>Small particle (EL30009B) ~20 <math>\mu\text{m}</math></th> </tr> </thead> <tbody> <tr> <td>24 h @ 31% RH</td> <td>0.01%</td> <td>0.02%</td> </tr> <tr> <td>72 h @ 31% RH</td> <td>0.05%</td> <td>0.07%</td> </tr> <tr> <td>7 days @ 31% RH</td> <td>0.07%</td> <td>0.07%</td> </tr> <tr> <td>24 h @ 74% RH</td> <td>0.03%</td> <td>0.03%</td> </tr> <tr> <td>72 h @ 74% RH</td> <td>0.03%</td> <td>0.05%</td> </tr> <tr> <td>7 days @ 74% RH</td> <td>0.03%</td> <td>0.06%</td> </tr> </tbody> </table>	Hygroscopicity @ 25 $^{\circ}\text{C}$	Large particle (EL3C106A) ~110 $\mu\text{m}$	Small particle (EL30009B) ~20 $\mu\text{m}$	24 h @ 31% RH	0.01%	0.02%	72 h @ 31% RH	0.05%	0.07%	7 days @ 31% RH	0.07%	0.07%	24 h @ 74% RH	0.03%	0.03%	72 h @ 74% RH	0.03%	0.05%	7 days @ 74% RH	0.03%	0.06%
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Compatibility	Good compatibility with RDX, HMX, CL-20 and HNS as well as some other energetic materials <sup>[3]</sup> , good compatibility with common construction materials <sup>[3]</sup> , slowly dissolves and decomposes in direct contact with water <sup>[11]</sup> , no dec. with 2-propanol <sup>[1,11]</sup> , compatible with RDX, HMX, NOL-130, CL-20, HNS, PYX, ZPP <sup>[11]</sup> , very slow dec. in water and is dependent on particle size <sup>[1]</sup>																					

Dent block test	Average dent = 0.037 in, average function time = 46 µs (24 mg ZPP pressed into P-N 2-300062 header with 1 ohm 0.0022 in stable ohm bridgewire @ 10 kpsi, materials loaded into stainless steel vessels with 7 mm wall thickness, pressed @ 10 kpsi, headers pressed into contact with output charges and sealed, units fired into 1 in Al blocks) <sup>[7]</sup> , average dent = 9.0 mils (@ average charge density = 1.26 g cm <sup>-3</sup> , 5 kpsi loading pressure, Al witness block) <sup>[9]</sup> , average dent = 13.2 mils (@ average charge density = 1.440 g cm <sup>-3</sup> , 10.0 kpsi loading pressure, Al witness block) <sup>[9]</sup> , average dent = 22.6 mils (@ average charge density = 1.38 g cm <sup>-3</sup> , 10.0 kpsi loading pressure, Al witness block) <sup>[9]</sup> , average dent = 31.7 mils (@ average charge density = 1.53 g cm <sup>-3</sup> , 20 kpsi loading pressure, Al witness block) <sup>[9]</sup> , average dent = 29.0 mils (@ average charge density = 1.77 g cm <sup>-3</sup> , 40.0 kpsi loading pressure, Al witness block) <sup>[9]</sup>
Thermal conductivity [Wm <sup>-1</sup> K <sup>-1</sup> ]	0.03 (free powder @ 29.5 °C) <sup>[1,11]</sup>

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 $\pm 2\%$ ; capacitor discharge Bruceton: used 0.1 or 1.0 mfd capacitor and 0.3 log unit voltage steps, data from ref. [11]:							
	Material	Aging	Bridge	Constant current			Cap. discharge	
	DBX-1	T = 0	Tophet	Mean (amps)	AF 99.9%	NF 0.1% (amps)	Mean (volts, mf)	Stored energy (mJ)
			0.001	0.252 $\pm$ 0.017	0.304	0.201	77.62 $\pm$ 0, 1.0	3.01
	DBX-1	T = 6 m	0.0005	0.106 $\pm$ 0.005	0.121	0.092	122.89 $\pm$ 6.42, 0.1	0.76
			0.001	0.244 $\pm$ 0.010	0.276	0.212	79.62 $\pm$ 10.94, 1.0	3.17
	DBX-1	T = 12 m	0.0005	0.105 $\pm$ 0.005	0.120	0.090	126.77 $\pm$ 7.82, 0.1	0.80
			0.001	0.228 $\pm$ 0.014	0.272	0.183	80.74 $\pm$ 1.08, 1.0	3.26
	DBX-1	controlled	0.0005	0.106 $\pm$ 0.007	0.127	0.086	138.23 $\pm$ 1.10, 0.1	0.96
			0.001	0.246 $\pm$ 0.028	0.332	0.160	85.31 $\pm$ 1.01, 1.0	3.64
			0.0005	0.110 $\pm$ 0.007	0.131	0.090	130.32 $\pm$ 1.09, 0.1	0.85
Hot wire initiation testing data from ref. [1]:	Hot wire initiation testing data from ref. [1]:							
	Material	Bridge (mm)	Constant current			Capacitor discharge		
	DBX-1	0.0254	Mean (mA)	All-fire 99.9%	No-fire 0.1%	Mean (volts, mF)		Stored energy (mJ)
			252 $\pm$ 17	304 mA	201 mA	77.62 $\pm$ 0, 1.0		3.01
	DBX-1	0.0127	106 $\pm$ 5	121 mA	92 mA	122.89 $\pm$ 1.05, 0.1		0.76

Priming ability test	<p>200 mg RDX pressed at 10 kpsi in 5,052 Al cup (0.295 in outer diameter, 0.262 in inner diameter, 2.985 in length), 0.01–10 g DBX-1 sample, plastic spacer to hold fuse, seal can at top of can, 1020 steel plate dent block (81 in outer diameter, 0.5 in thick), PMMA holder (1.25 in long, 1 in outer diameter)<sup>[11]</sup>:</p> <table border="1"> <thead> <tr> <th>Sample</th><th colspan="2">Priming ability test (Bruceton analysis)</th></tr> <tr> <th></th><th>Level 50<sub>0</sub> (g)</th><th><math>\sigma_0</math></th></tr> </thead> <tbody> <tr> <td>DBX-1, T = 0 month</td><td>0.0263</td><td>0.0066</td></tr> <tr> <td>DBX-1, T = 6 months</td><td>0.0279</td><td>0.0059</td></tr> <tr> <td>DBX-1, T = 12 months</td><td>0.0256</td><td>0.0067</td></tr> <tr> <td>DBX-1, T = 12 months (unaged)</td><td>0.0250</td><td>0.0108</td></tr> </tbody> </table> <p>Loose charge of 0.01 g DBX-1 insufficient to cause detonation of 200 mg RDX charge<sup>[1]</sup>, level 500% – 26.3 ± 6.6 mg (from larger loads of 0.025 or 0.040 g)<sup>[11]</sup></p>	Sample	Priming ability test (Bruceton analysis)			Level 50 <sub>0</sub> (g)	$\sigma_0$	DBX-1, T = 0 month	0.0263	0.0066	DBX-1, T = 6 months	0.0279	0.0059	DBX-1, T = 12 months	0.0256	0.0067	DBX-1, T = 12 months (unaged)	0.0250	0.0108						
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Cook-off test	<p>F-18 directed tests – cook-off testing data from ref.<sup>[11]</sup>:</p> <table border="1"> <thead> <tr> <th>Time (h)</th> <th>DBX-1/HNS-1 (°F/dent – mils)</th> </tr> </thead> <tbody> <tr> <td>1 (MIL-I-23659)</td> <td>500/fired 475/no fire (31 mils)</td> </tr> <tr> <td>12 (MIL-I-23659)</td> <td>450/fired 400/no fire (31 mils)</td> </tr> <tr> <td>50</td> <td>340/no fire (30 mils)</td> </tr> <tr> <td>Untreated</td> <td>29 mils</td> </tr> </tbody> </table>	Time (h)	DBX-1/HNS-1 (°F/dent – mils)	1 (MIL-I-23659)	500/fired 475/no fire (31 mils)	12 (MIL-I-23659)	450/fired 400/no fire (31 mils)	50	340/no fire (30 mils)	Untreated	29 mils														
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Laser ignition	mm samples in glass capillaries initiate using Nd:YAG laser with $\lambda = 1,064$ nm and nominal pulse width of 12 ns coupled to the sample with fiber optics <sup>[12]</sup>																								
Dead pressing	Not dead-pressed @ 275.8 MPa loading pressure <sup>[1]</sup>																								
$\Delta H_{dec}$ [J/g]	1967 (DSC @ 20 K/min) <sup>[1]</sup>																								
pH	6.69 (suspension of 0.52 g DBX-1 in 100 mL deionized water) <sup>[1]</sup>																								

	<b>DBX-1<sup>[1]</sup></b>
Chemical formula	C <sub>2</sub> Cu <sub>2</sub> N <sub>10</sub> O <sub>4</sub>
Molecular weight [g mol <sup>-1</sup> ]	355.20
Crystal system	Monoclinic
Space group	p2 <sub>1</sub> /c
a [Å]	10.513(2)
b [Å]	10.280(2)
c [Å]	9.402(2)
α [°]	90
β [°]	116.032(3)
γ [°]	90
V [Å <sup>3</sup> ]	913.0(4)
Z	4
ρ <sub>calc</sub> [g cm <sup>-3</sup> ]	2.584
T [K]	113

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- [6] K. D. Oyler, *Green Primary Explosives*, Ch. 5 in *Green Energetic Materials*, T. Brinck (ed.), Wiley, **2014**.
- [7] J. W. Fronabarger, M. D. Williams, W. B. Sanborn, *Lead-Free Primary Explosive Composition and Method of Preparation*, International Patent WO 2008/048351 A2, 24th April **2008**.
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## Cupric azide

Name [German, acronym]: Copper(II) azide\* [kupfer(II)-azid]

Main (potential) use: Primary explosive for detonators

Structural formula:



\* “Basic copper azide” refers to copper azides of the type  $\text{Cu}(\text{N}_3)_2 \bullet \text{Cu}(\text{OH})_2$ ,  $\text{Cu}(\text{N}_3)_2 \bullet 2\text{Cu}(\text{OH})_2$  or  $\text{Cu}(\text{N}_3)_2 \bullet 3\text{Cu}(\text{OH})_2$ <sup>[2]</sup>

	<b>Cu(N<sub>3</sub>)<sub>2</sub></b>		
Formula	CuN <sub>6</sub>		
Molecular mass [g mol <sup>-1</sup> ]	147.59		
Appearance at RT	Dark brown-black crystalline solid <sup>[1,3]</sup> , brown-red needles <sup>[2]</sup> , dark green needles <sup>[2]</sup> , black-brown solid with red shine <sup>[3]</sup> , long prismatic greenish black needles <sup>[5]</sup> , black-brown solid <sup>[7]</sup>		
IS [J]	1 cm (1 kg mass, crystals) <sup>[1,3]</sup> , 9 cm (500 g mass, H <sub>50%</sub> , crystals) <sup>[1]</sup> , 2 cm (1 kg mass, amorphous) <sup>[1,3]</sup> , <1 cm (1 kg mass, green copper azide) <sup>[3]</sup> , 1 cm (1 kg mass, black crystalline) <sup>[3]</sup> , 2 cm (1 kg mass, amorphous) <sup>[3]</sup> , drop weight = 600 mg, upper limit = 70 cm, lower limit = 70 cm <sup>[4]</sup> , explodes with high brisance even under water <sup>[7]</sup> , explosion by impact is very violent and spontaneous explosion has been reported <sup>[10]</sup> , good crystals are considerably more sensitive than the powder <sup>[10]</sup>		
Impact sensitivity of different particle sizes of cupric azide <sup>[1]</sup> :			
Probability of initiation (%)	Height (cm)		
	Crystal mesh 150	Precipitated Sample	Crystal mesh 240
10	~ 13	—	~ 39
20	—	~ 39	—
30	~ 26	~ 46	~ 51
40	—	—	—
50	~ 38	~ 51	~ 59
60	~ 45	~ 58	~ 64
70	~ 47	—	—
80	~ 51	~ 64	~ 70
90	—	~ 70	~ 77
100	~ 65	~ 78	—

	Ball and disk IS <sup>[8]</sup> :		
	Explosive		Height for 50% reactions (cm)
	Monobasic cupric azide, $\text{Cu}(\text{N}_3)_2 \bullet \text{Cu}(\text{OH})_2$		0.170
	Dibasic cupric azide, $\text{Cu}(\text{N}_3)_2 \bullet 2\text{Cu}(\text{OH})_2$		0.057
FS [N]	Explodes on wiping the crystals from paper using a soft brush <sup>[3]</sup> , explodes with high brisance even under water <sup>[7]</sup> , loosening solid from filter paper caused initiation <sup>[10]</sup> , spontaneous explosion has been reported <sup>[10]</sup> , good crystals are considerably more sensitive than the powder <sup>[10]</sup>		
	Emery paper FS <sup>[8]</sup> :		
	Explosive		Velocity of stroke for 50% reactions (ft/s)
	Monobasic cupric azide, $\text{Cu}(\text{N}_3)_2 \bullet \text{Cu}(\text{OH})_2$		0.124
ESD [J]	0.1–0.2 mJ <sup>[1]</sup> , 1–2 ergs (min. energy) <sup>[2]</sup> , explodes in the microjoule range <sup>[5]</sup> , good crystals are considerably more sensitive than the powder <sup>[10]</sup>		
N [%]	56.94		
$\Omega(\text{CO}_2)$ [%]			
$T_{\text{dec.}}$ [°C]	178–240 with exothermic peak max. @ 216 °C (DSC @ 10 °C/min) <sup>[6]</sup> , 175 °C mass loss = 12.6%, 216 °C mass loss = 43.67% (TG-DTG @ 10 °C/min) <sup>[6]</sup>		
$\rho$ [g cm <sup>-3</sup> ]	2.2–2.5 <sup>[1]</sup> , 2.58 <sup>[1]</sup> , $2.058 \pm 0.04$ <sup>[2]</sup> , $d_{25^\circ} = 2.20$ (pseudomorphic) <sup>[3]</sup> , $d_{25^\circ} = 2.25$ (crystalline) <sup>[3]</sup> , 2.604 (X-ray) <sup>[3]</sup> , 2.58 (flootation in 1-bromonaphthalene-diiodomethane mixtures) <sup>[5]</sup>		
Heat of formation	587 kJ mol <sup>-1</sup> ( $\Delta_f H$ ) <sup>[1]</sup> , 140.4 kcal/mol (standard enthalpy of form., @ 25 °C, cryst.) <sup>[9]</sup>		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{\text{ex}} U^\circ$ [kJ kg <sup>-1</sup> ]			
$T_{\text{ex}}$ [K]			
$p_{\text{C-J}}$ [kbar]			
VoD [m s <sup>-1</sup> ]			5,000–5,500 (depending on $\rho$ ) <sup>[3]</sup>

$V_0$ [L kg <sup>-1</sup> ]			456 <sup>[3]</sup>	
Trauzl test [cm <sup>3</sup> , % TNT]	115 (netto, 10 g Cu(N <sub>3</sub> ) <sub>2</sub> ) <sup>[3]</sup>			
Initiation efficiency	0.0004 g brings nitropentaerythrit to detonation <sup>[3]</sup> , exceptionally powerful initiator <sup>[10]</sup>			
5 s explosion $T$ [°C] Explosion $T$ [°C] Ignition $T$ [°C]	202–205 (depending on the heating) <sup>[3]</sup> , 202 <sup>[7]</sup> 201 (very violent, 5 °C/min) <sup>[2]</sup>			
Thermal stability	Crystals are stable in air <sup>[5]</sup> , very explosive even when moist <sup>[10]</sup>			
Vapor pressure [atm. @ °C]	Nonvolatile <sup>[7]</sup>			
Response to open flame	Detonates <sup>[1,2]</sup> , wet Cu(N <sub>3</sub> ) <sub>2</sub> does not ignite in flame <sup>[3]</sup>			
Solubility [g/mL]	H <sub>2</sub> O = slightly soluble <sup>[1]</sup> , insoluble in most common organic solvents <sup>[1]</sup> , 0.080 g/L H <sub>2</sub> O @ RT <sup>[3]</sup> , 0.3178 g/L of 2% aq. NH <sub>3</sub> @ RT <sup>[3]</sup> , insoluble in EtOH <sup>[3]</sup> , very poor solubility in water and even poorer solubility in organic solvents (except those that form complexes) <sup>[3]</sup> , easily soluble in some dilute acids including acetic acid <sup>[3]</sup> soluble in and forms complexes with NH <sub>3</sub> , alkali azides, ammonium azide and aliphatic amines in aqueous or alcohol soln. <sup>[3]</sup> , insoluble in water and organic solvents <sup>[7]</sup> , 0.0080 g/100 g water @ 15 °C <sup>[9]</sup>			
Hygroscopicity	Crystals are stable in air <sup>[5]</sup>			
Photosensitivity	Not light sensitive <sup>[1,7]</sup> , crystals disintegrate rapidly in X-ray radiation (Cu–K <sub>α</sub> ) <sup>[5]</sup>			
Compatibility	No effect with HN <sub>3</sub> vapor <sup>[2]</sup> , hydrolyzes (copper strip test) rapidly to Cu(N <sub>3</sub> ) <sub>2</sub> Cu(OH) <sub>2</sub> with liberation of HN <sub>3</sub> <sup>[2]</sup> , hydrolyzes in boiling H <sub>2</sub> O <sup>[3]</sup> , dec. in strong bases <sup>[3]</sup> , dec. in conc. H <sub>2</sub> SO <sub>4</sub> <sup>[3]</sup> , stable in closed vessel <sup>[3]</sup> , hydrolyzes in boiling water <sup>[3]</sup> , dec. on heating in air <sup>[3]</sup> , aqueous hydrazine causes reduction <sup>[3]</sup> , hydrolyzes in boiling water <sup>[7]</sup>			
$\Delta H_{dec}$ [J/g]	3,116.86 (DSC) <sup>[6]</sup>			
Enthalpy of soln. [kcal/mol]	3.59 <sup>[9]</sup>			

	Cu(N <sub>3</sub> ) <sub>2</sub> <sup>[2,3]</sup>	Cu(N <sub>3</sub> ) <sub>2</sub> <sup>[2]</sup>	Cu(N <sub>3</sub> ) <sub>2</sub> <sup>[5]</sup>	Cu(N <sub>3</sub> ) <sub>2</sub> <sup>[9]</sup>
Chemical formula	CuN <sub>6</sub>	CuN <sub>6</sub>	CuN <sub>6</sub>	CuN <sub>6</sub>

Molecular weight [g mol <sup>-1</sup> ]				
Crystal system	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic
Space group	<i>Pbnm</i> or <i>Pbn2</i> <sub>1</sub>	<i>Pbnm</i> or <i>Pbn2</i> <sub>1</sub>	<i>Pbnm</i>	
<i>a</i> [Å]	9.226	9.12	9.084 ± 0.003	9.23
<i>b</i> [Å]	13.225	13.53	13.454 ± 0.002	13.23
<i>c</i> [Å]	3.068	3.09	3.079 ± 0.001	3.07
$\alpha$ [°]	90	90	90	90
$\beta$ [°]	90	90	90	90
$\gamma$ [°]	90	90	90	90
<i>V</i> [Å <sup>3</sup> ]			376.3 ± 0.3	
<i>Z</i>	4	4	4	8
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	2.57 (2.604 <sup>[3]</sup> )		2.604	
<i>T</i> [K]			25 °C	
		X-ray powder data	Long prismatic greenish black needles which show extremely strong pleochroism	

Crystals are strongly pleochroic; appear brown-black when the electric vector is parallel to the length of the crystals; green-black crystals<sup>[2]</sup>; Cu(N<sub>3</sub>)<sub>2</sub> is orthorhombic<sup>[6]</sup>

- [1] R. Matyáš, J. Pachman, *Primary Explosives*, Springer Verlag, 2013.
- [2] *Proc. Symp. on Lead and Copper Azides*, E.R.D.E., 25th–26th October 1966, Essex, UK, AD-A011026.
- [3] M. Straumanis, A. Cirulis, *ZAAC*, **1943**, 251, 315–331.
- [4] C. Zhang, X. C. Wang, H. Huang, *Computational Treatment of the Structure-Sensitivity Relationships of Explosives*, ICT 2008, Karlsruhe, Germany, pp. 99-1–99-9.
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- [6] N. Li, J.-B. Xu, Y.-H. Ye, R.-Q. Shen, Y. Hu, *Chinese J. Explosives, Propellants*, **2015**, 38, 63–66.
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- [8] L. Avrami, R. Hutchinson, *The Sensitivity to Impact and Friction*, Ch. 4 in *Energetic Materials 2: Technology of the Inorganic Azides*, H. D. Fair, R. F. Walker (eds.), Plenum Press, 1977.
- [9] B. L. Evans, A. D. Yoffe, P. Gray, *Chem. Revs.*, **1959**, 59, 515–568.
- [10] *Bretherick's Handbook of Reactive Chemical Hazards*, vol. 1, 7th edn., P. G. Urben (ed.), Elsevier, 2007, p. 1561.

## Cuprous azide

Name [German, acronym]: Copper(I) azide [kupfer(I)-azid]

Main (potential) use: primary explosive

Structural formula:



	<b>CuN<sub>3</sub></b>																								
Formula	Cu <sub>2</sub> (N <sub>3</sub> ) <sub>2</sub>																								
Molecular mass [g mol <sup>-1</sup> ]	211.14																								
Appearance at RT	White crystalline solid <sup>[1]</sup> , yellow plates <sup>[2]</sup> , white crystalline solid, but usually obtained as gray-green powder <sup>[7]</sup> , yellow-green needles and plates (recryst.) <sup>[10]</sup> CuN <sub>3</sub> form I: white-gray <sup>[2]</sup> , form-II: white <sup>[2]</sup>																								
IS [J]	<p>H<sub>50%</sub> = 16 cm (500 g mass)<sup>[1]</sup>, H<sub>50%</sub> = 10 cm (130 g ball)<sup>[1]</sup>, H<sub>40%</sub> = 10 cm (130 g ball)<sup>[1]</sup>, H<sub>80%</sub> = 12.5 cm (130 g ball)<sup>[1]</sup>, H<sub>40%</sub> = 10 cm (Form-I, 130 g ball, FOA ball impact test)<sup>[2]</sup>, H<sub>80%</sub> = 12.5 cm (Form-II, 130 g ball, FOA ball impact test)<sup>[2]</sup>, extremely sensitive<sup>[7]</sup>, very highly impact sensitive<sup>[11]</sup>  Work = 2.66 kg m cm<sup>2</sup>, drop weight = 600 mg, upper limit = 125 cm, lower limit = 70 cm<sup>[4]</sup></p> <p>Ball drop apparatus, <math>\frac{7}{8}</math> in ball, 15 trials at each height, % samples reacting<sup>[8]</sup>:</p> <table border="1"> <thead> <tr> <th>Height (in)</th> <th>Crystalline sample (150 mesh)</th> <th>Precipitated sample</th> <th>Crystalline sample (240 mesh)</th> </tr> </thead> <tbody> <tr> <td>5</td> <td>10</td> <td></td> <td></td> </tr> <tr> <td>10</td> <td>25</td> <td></td> <td></td> </tr> <tr> <td>15</td> <td>50</td> <td>20</td> <td>10</td> </tr> <tr> <td>20</td> <td>90</td> <td>50</td> <td>35</td> </tr> <tr> <td>25</td> <td>&gt;90</td> <td>90</td> <td>65</td> </tr> </tbody> </table>	Height (in)	Crystalline sample (150 mesh)	Precipitated sample	Crystalline sample (240 mesh)	5	10			10	25			15	50	20	10	20	90	50	35	25	>90	90	65
Height (in)	Crystalline sample (150 mesh)	Precipitated sample	Crystalline sample (240 mesh)																						
5	10																								
10	25																								
15	50	20	10																						
20	90	50	35																						
25	>90	90	65																						
FS [N]	30 g load, 50% explosion probability <sup>[1]</sup> , 40 g load, 80% explosion probability <sup>[1]</sup> , 30 g load, 50% explosion frequency (form-I, Julius-Peters machine) <sup>[2]</sup> , 40 g load, 80% explosion frequency (form-I, Julius-Peters machine) <sup>[2]</sup> , extremely sensitive <sup>[7]</sup>																								
ESD [J]	0.1–0.2 μJ <sup>[1]</sup> , exploded at minimum energy value obtainable with apparatus (1 m) <sup>[2]</sup> , 1–10 μJ (est. min. energy required to cause explosion) <sup>[2]</sup> , 1–2 ergs (min. energy, completes) <sup>[2]</sup>																								
N [%]	39.80																								

$\Omega(\text{CO}_2)$ [%]			
$T_{\text{m.p.}}$ [°C]	~205 (dec.) <sup>[10]</sup>		
$T_{\text{dec.}}$ [°C]	205 <sup>[11]</sup>		
$\rho$ [g cm <sup>-3</sup> ]	3.26 (pycnometer) <sup>[1,5]</sup> , 3.34 (X-ray) <sup>[1]</sup>		
Heat of formation	281 kJ mol <sup>-1</sup> ( $\Delta_f H$ ) <sup>[1]</sup> , 67.23 kcal/mol (standard enthalpy of form., @ 25 °C, exptl.) <sup>[10]</sup> , 253.1 kJ/mol ( $\Delta H^o_f$ ) <sup>[11]</sup>		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^o$ [kJ kg <sup>-1</sup> ]			
$T_{\text{ex}}$ [K]			
$p_{\text{CJ}}$ [kbar]			
VoD [m s <sup>-1</sup> ]			
$V_0$ [L kg <sup>-1</sup> ]			
Critical diameter [cm]	Can detonate in very thin layers; detonation propagates in layers thicker than 0.85 mg/cm <sup>2</sup> <sup>[2]</sup>		
5 s explosion $T$ [°C]	~216 <sup>[1]</sup> , 197 (10 mg sample, minimum $T$ = 174 °C) <sup>[9]</sup>		
Ignition $T$ [°C]	192 (very violent, 5 °C/min) <sup>[2]</sup> , 478 K <sup>[6]</sup> , 447 K (174 °C) <sup>[6]</sup>		
Explosion $T$ [°C]	220 <sup>[7]</sup> , 205 (2 sec, 7 mg sample) <sup>[9]</sup>		
Response to open flame	Detonates <sup>[1]</sup> , detonates (form-I and form-II) <sup>[2]</sup>		
Solubility [g/mL]	Practically insoluble in H <sub>2</sub> O and most common organic solvents <sup>[1,7]</sup> , 0.0075 g/L H <sub>2</sub> O @ RT <sup>[3]</sup> , 0.2897 g/L of 2% aq. NH <sub>3</sub> @ RT <sup>[3]</sup>		
Photosensitivity	Photosensitive in sunlight <sup>[1]</sup> , form-I is photosensitive and form-II is photosensitive <sup>[2]</sup> , photosensitive, exposure to light forms red solid <sup>[7]</sup> , critical light energy required for ignition by a 50 μs light flash = 12 J (total energy) <sup>[10]</sup>		
Compatibility	Converted to black Cu(N <sub>3</sub> ) <sub>2</sub> with HN <sub>3</sub> vapor <sup>[2]</sup> , hydrolyzes (copper strip test) rapidly to Cu(N <sub>3</sub> ) <sub>2</sub> Cu(OH) <sub>2</sub> with no liberation of HN <sub>3</sub> <sup>[2]</sup> , Cu <sup>+</sup> is oxidized on exposure to atmospheric oxygen <sup>[7]</sup>		
Sensitiveness	2.66 N cm <sup>2</sup> (work) <sup>[6]</sup>		
Refractive index	>1.81 <sup>[10]</sup>		
Dielectric constant, $k$	9.3 (low frequency, frequency = 2–4.5 mc/s) <sup>[10]</sup>		

	$\text{CuN}_3^{[5,6]}$	$\text{CuN}_3^{[10]}$
Chemical formula	$\text{CuN}_3$	$\text{CuN}_3$
Molecular weight [g mol <sup>-1</sup> ]		
Crystal system	Tetragonal	Tetragonal
Space group	$I4_1/a$	
$a$ [\AA]	$8.65(3) \pm 0.01$	8.65
$b$ [\AA]	$8.65(3) \pm 0.01$	8.65
$c$ [\AA]	5.594(4) ± 0.01	5.59
$\alpha$ [°]	90	90
$\beta$ [°]	90	90
$\gamma$ [°]	90	90
$V$ [\AA <sup>3</sup> ]		
$Z$	8	8
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	3.34	
$T$ [K]		

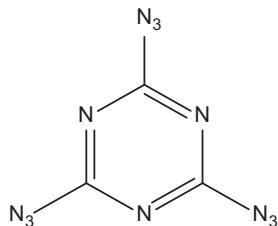
- [1] R. Matyáš, J. Pachman, *Primary Explosives*, Springer Verlag, 2013.
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- [5] H. Wilsdorf, *Acta Cryst.*, **1948**, 1, 115–118.
- [6] M. Cartwright, J. Wilkinson, *Propellants, Explosives, Pyrotechnics*, **2010**, 35, 326–332.
- [7] *Energetic Materials 1: Physics and Chemistry of the Inorganic Azides*, H. D. Fair, R. F. Walker (eds.), Plenum Press, 1977.
- [8] L. Avrami, R. Hutchinson, *The Sensitivity to Impact and Friction*, Ch. 4 in *Energetic Materials 2: Technology of the Inorganic Azides*, H. D. Fair, R. F. Walker (eds.), Plenum Press, 1977.
- [9] L. Avrami, J. Haberman, *Sensitivity to Heat and Nuclear Radiation*, Ch. 6 in *Energetic Materials 2: Technology of the Inorganic Azides*, H. D. Fair, R. F. Walker (eds.), Plenum Press, 1977.
- [10] B. L. Evans, A. D. Yoffe, P. Gray, *Chem. Revs.*, **1959**, 59, 515–568.
- [11] *Bretherick's Handbook of Reactive Chemical Hazards*, vol. 1, 7th edn., P. G. Urben (ed.), Elsevier, 2007, p. 1564.

## Cyanuric triazide

Name [German, acronym]: 1,3,5-Triazido-2,4,6-triazine, cyanuric triazide, triazine triazide [cyanurtriazid, TTA, TAT]

Main (potential) use: Replacement for lead azide in stab detonators<sup>[1]</sup>, possible LA/LS replacement in initiator mixtures, patented in 1921 as a detonating explosive used in detonators<sup>[18]</sup>

Structural formula:



	TTA																																															
Formula	C <sub>3</sub> N <sub>12</sub>																																															
Molecular mass [g mol <sup>-1</sup> ]	204.12																																															
Appearance at RT	Colorless crystals on recryst. from EtOH <sup>[17]</sup> , white crystalline solid <sup>[19]</sup>																																															
IS [J]	0.15 <sup>[2]</sup> , 1.3 <sup>[7]</sup> , 0.7 (7 cm, 1 kg mass, 20 mg sample, B.M.) <sup>[8]</sup> , 0.34 (needles of 0.04–0.2 mm diameter, average length = 0.1 mm, small impact machine, 7 cm, 0.5 kg mass) <sup>[10]</sup> , 0.18 (B.M., 0.9 cm, 2 kg mass) <sup>[10]</sup> , 0.69 (7 cm, 1 kg mass, B.M.) <sup>[10]</sup> , 25.4 cm (ball drop impact) <sup>[10]</sup> , H <sub>50</sub> = 6.2 cm (type 12 tool) <sup>[10]</sup> , H <sub>50</sub> = 6.2 cm <sup>[17]</sup>																																															
	Influence of grit on IS <sup>[23]</sup> :																																															
	<table border="1"> <thead> <tr> <th rowspan="2">Grit</th> <th rowspan="2">Hardness (mols.)</th> <th rowspan="2">Mpt. (°C)</th> <th colspan="2">Explosion efficiency (45 g, 30 cm)</th> </tr> <tr> <th>No.</th> <th>%</th> </tr> </thead> <tbody> <tr> <td>Nil</td> <td>—</td> <td>—</td> <td>0/20</td> <td>0</td> </tr> <tr> <td>Silver nitrate</td> <td>2–3</td> <td>212</td> <td>0/5</td> <td>0</td> </tr> <tr> <td>Silver bromide</td> <td>2–3</td> <td>434</td> <td>0/5</td> <td>0</td> </tr> <tr> <td>Lead nitrate</td> <td>2–3</td> <td>470</td> <td>0/5</td> <td>0</td> </tr> <tr> <td>Lead chloride</td> <td>2–3</td> <td>501</td> <td>0/10</td> <td>0</td> </tr> <tr> <td>Borax</td> <td>3–4</td> <td>560</td> <td>5/5</td> <td>100</td> </tr> <tr> <td>Bismuthinite</td> <td>2–2.5</td> <td>685</td> <td>5/5</td> <td>100</td> </tr> <tr> <td>Chalcocite</td> <td>3–3.5</td> <td>1100</td> <td>5/5</td> <td>100</td> </tr> </tbody> </table>	Grit	Hardness (mols.)	Mpt. (°C)	Explosion efficiency (45 g, 30 cm)		No.	%	Nil	—	—	0/20	0	Silver nitrate	2–3	212	0/5	0	Silver bromide	2–3	434	0/5	0	Lead nitrate	2–3	470	0/5	0	Lead chloride	2–3	501	0/10	0	Borax	3–4	560	5/5	100	Bismuthinite	2–2.5	685	5/5	100	Chalcocite	3–3.5	1100	5/5	100
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	<p>IS of molten cyanuric azide (<math>T = 110^\circ\text{C}</math>)<sup>[23]</sup>:</p> <table border="1"> <thead> <tr> <th rowspan="2">Type of striker</th><th rowspan="2">Energy of impact</th><th colspan="2">Explosion efficiency</th></tr> <tr> <th>No.</th><th>%</th></tr> </thead> <tbody> <tr> <td>Brass cavity</td><td>295 g, 20 cm</td><td>5/5</td><td>100</td></tr> <tr> <td>Brass bored cavity</td><td>295 g, 20 cm</td><td>0/5</td><td>0</td></tr> </tbody> </table> <p>IS of molten cyanuric azide using smooth curved striker or a curved striker containing a cavity<sup>[23]</sup>:</p> <table border="1"> <thead> <tr> <th rowspan="2">Type of striker</th><th rowspan="2">Energy of impact</th><th colspan="2">Explosion efficiency</th></tr> <tr> <th>No.</th><th>%</th></tr> </thead> <tbody> <tr> <td rowspan="3">Cavity</td><td>295 g, 20 cm</td><td>5/5</td><td>100</td></tr> <tr> <td>195 g, 20 cm</td><td>2/10</td><td>20</td></tr> <tr> <td>60 g, 20 cm</td><td>0/10</td><td>0</td></tr> <tr> <td rowspan="4">Smooth</td><td>295 g, 20 cm</td><td>5/5</td><td>100</td></tr> <tr> <td>195 g, 20 cm</td><td>5/5</td><td>100</td></tr> <tr> <td>60 g, 20 cm</td><td>5/5</td><td>100</td></tr> <tr> <td>60 g, 10 cm</td><td>2/10</td><td>20</td></tr> </tbody> </table>	Type of striker	Energy of impact	Explosion efficiency		No.	%	Brass cavity	295 g, 20 cm	5/5	100	Brass bored cavity	295 g, 20 cm	0/5	0	Type of striker	Energy of impact	Explosion efficiency		No.	%	Cavity	295 g, 20 cm	5/5	100	195 g, 20 cm	2/10	20	60 g, 20 cm	0/10	0	Smooth	295 g, 20 cm	5/5	100	195 g, 20 cm	5/5	100	60 g, 20 cm	5/5	100	60 g, 10 cm	2/10	20
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FS [N]	<p>0.1 N pistil load<sup>[1]</sup>, &lt;0.5<sup>[7]</sup>; no go at -, go at 10 N (nonrecrystallized)<sup>[10]</sup>, no go at 10, go at 20 (recrystallized)<sup>[10]</sup>, &lt;0.5 kg (BAM)<sup>[10]</sup>, &lt;0.5 kg<sup>[17]</sup></p> <p>BAM FS<sup>[21]</sup>:</p> <table border="1"> <thead> <tr> <th rowspan="2">Reaction observed</th><th colspan="4">Load on porcelain peg (g)</th></tr> <tr> <th>10</th><th>20</th><th>30</th><th>40</th></tr> </thead> <tbody> <tr> <td>No reaction</td><td>2</td><td>1</td><td>1</td><td>0</td></tr> <tr> <td>Ignition</td><td>0</td><td>0</td><td>0</td><td>0</td></tr> <tr> <td>Detonation</td><td>4</td><td>5</td><td>5</td><td>6</td></tr> </tbody> </table>	Reaction observed	Load on porcelain peg (g)				10	20	30	40	No reaction	2	1	1	0	Ignition	0	0	0	0	Detonation	4	5	5	6																			
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ESD [J]	1.2 mJ <sup>[6]</sup> ; nonrecrystallized no go at 31 mJ <sup>[10]</sup> , recrystallized no go at 1.2 mJ <sup>[10]</sup> , <0.36 (spark sensitivity) <sup>[10,17]</sup>																																											
N [%]	82.35																																											
$\Omega(\text{CO}_2)$ [%]	-47.0																																											
$T_{\text{m.p.}}$ [ $^\circ\text{C}$ ]	94 <sup>[3,6–8,17,18,22]</sup> , (sublimation begins above 30 $^\circ\text{C}$ <sup>[6]</sup> ), 367.4 K (endo peak min., DSC @ 2 K/min Ar purge flow) <sup>[20]</sup> , 94.5 <sup>[23]</sup>																																											
$T_{\text{b.p.}}$ [ $^\circ\text{C}$ ]	267.7 (@ $P_s = 1.013 \times 10^5$ Pa, calcd. from Clausius–Clapeyron eqn.); however, $T_b$ is unattainable due to very high rate of TTA dec. <sup>[20]</sup>																																											
$T_{\text{dec.}}$ [ $^\circ\text{C}$ ]	180 (DSC) <sup>[3]</sup> , >100 <sup>[6]</sup> (ignition temperature = ~205 $^\circ\text{C}$ <sup>[6]</sup> ), 187 <sup>[7]</sup> , >100 <sup>[8,18]</sup> , 187 (DSC, fast dec.) <sup>[10]</sup>																																											

$\rho$ [g cm <sup>-3</sup> ]	1.54 (@ 286.15 K) <sup>[2]</sup> , 1.73 (crystal) <sup>[6]</sup> , 1.54 <sup>[8]</sup> , 1.736 (crystal) <sup>[17]</sup> , 1.54 (crystal) <sup>[8]</sup> , 1.4 (loading density @ 200 atm.) <sup>[8]</sup> , 1.5 (loading density @ 800 atm.) <sup>[8]</sup>		
Heat of formation	914.6 ( $\Delta_f H^\circ$ ) <sup>[4]</sup> , 4,561–4,761 kJ/kg <sup>[8]</sup> , 4,480.7 ( $\Delta_f H^\circ$ ) <sup>[4]</sup> , 4,489.2 kJ/kg (enthalpy of form.) <sup>[1]</sup> , 1,100 kcal/kg <sup>[14]</sup> , –1,090 to –1,138 cal/g <sup>[8]</sup> , 218.6 kcal/mol ( $\Delta_f H^\circ$ , exptl.) <sup>[16]</sup> , 1,053 kJ/mol ( $\Delta_f H$ ) <sup>[17]</sup>		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{ex} U^\circ$ [kJ kg <sup>-1</sup> ]	4,141		
$T_{ex}$ [K]	3,536	3,956 (@ 1.15 g cm <sup>-3</sup> , calcd.) <sup>[16]</sup>	
$p_{CJ}$ [kbar]	226.3	88.9 (@ 1.15 g cm <sup>-3</sup> , calcd.) <sup>[16]</sup>  228.7 (@ 1.697 g cm <sup>-3</sup> ) <sup>[5]</sup>	
VoD [m s <sup>-1</sup> ]	7,866 (@ 1.73 g cm <sup>-3</sup> , $\Delta_f H = 9.5$ kJ mol <sup>-1</sup> )	7,300 (@ 1.5 g cm <sup>-3</sup> ) <sup>[6]</sup> ~6,900 (@ 1.5 g cm <sup>-3</sup> ) <sup>[9]</sup>  5,650 (@ 1.15 g cm <sup>-3</sup> ) <sup>[4]</sup>  5,650 (@ 1.15 g cm <sup>-3</sup> , calcd.) <sup>[16]</sup>  1,820 ft/s (@ 1.1 g/mL) <sup>[19]</sup>	5,600 (@ 1.15 g cm <sup>-3</sup> ) <sup>[4,16]</sup>  5,550–5,600 (@ 1.15 g cm <sup>-3</sup> , 0.3 in charge diameter) <sup>[8]</sup>  5,500 (@ 1.02 g cm <sup>-3</sup> , unconfined) <sup>[10]</sup>  5,440–5,650 (@ 1.15 g cm <sup>-3</sup> ) <sup>[10]</sup>  7,500 (@ 1.54 g cm <sup>-3</sup> ) <sup>[13]</sup>  5,545 (@ 1.15 g cm <sup>-3</sup> , detonator capsules, 7.7 mm internal diameter, compressed to usual $\rho$ of commercial detonators, Kast) <sup>[18]</sup>
$V_0$ [L kg <sup>-1</sup> ]	719		

Trauzl test [cm <sup>3</sup> , % TNT]	140–145% TNT <sup>[13]</sup> , 415 cm <sup>3</sup> (10 g sample) <sup>[10]</sup> , 138% TNT <sup>[10]</sup> , 140% <sup>[10]</sup>																
Sand test [g]	32.2 g (200 g bomb) <sup>[8]</sup> , 99% TNT <sup>[13]</sup> , 32.2 g (67% TNT, 264% MF) <sup>[10]</sup>																
	<table border="1"> <thead> <tr> <th>Weight of cyanuric azide (g)</th> <th>Weight of sand crushed (g)<sup>[18]</sup></th> </tr> </thead> <tbody> <tr> <td>0.050</td> <td>2.6</td> </tr> <tr> <td>0.100</td> <td>4.8</td> </tr> <tr> <td>0.200</td> <td>12.2</td> </tr> <tr> <td>0.400</td> <td>33.2</td> </tr> <tr> <td>0.600</td> <td>54.4</td> </tr> <tr> <td>0.800</td> <td>68.9</td> </tr> <tr> <td>1.000</td> <td>78.6</td> </tr> </tbody> </table>	Weight of cyanuric azide (g)	Weight of sand crushed (g) <sup>[18]</sup>	0.050	2.6	0.100	4.8	0.200	12.2	0.400	33.2	0.600	54.4	0.800	68.9	1.000	78.6
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1.000	78.6																
Ballistic mortar test	145% TNT <sup>[13]</sup>																
Initiation sensitivity	Hot wire: cracks @ 20–50 °C <sup>[10]</sup> , explodes @ 75 °C <sup>[10]</sup> , does not explode when initiated by hot wire (unconfined, thin layers) <sup>[23]</sup>																
Initiation efficiency	<p>0.20 g LA minimum detonating charge<sup>[8]</sup>, 0.10 g tetryl minimum detonating charge<sup>[8]</sup>, capable of initiating explosive D<sup>[8]</sup></p> <p>Minimum initiating charge of cyanuric azide required (g) (0.4 g high explosive loaded into detonator capsules, pressed down, initiator added, covered with short reinforcing cap, pressed with 200 atm per square inch pressure; size of initiating charge was reduced until further reduction resulted in failure of high explosive to detonate)<sup>[18]</sup>: TNT – 0.10 g cyanuric azide, picric acid – 0.05 g cyanuric azide, tetryl – 0.04 g cyanuric azide, tetranitroaniline – 0.09 g cyanuric azide, ammonium picrate – 0.15 g cyanuric azide<sup>[18]</sup></p> <p>Minimal charge in a no. 8 detonator in priming ability test toward tetryl was 0.02 g<sup>[6]</sup></p>																
5 s explosion T [°C] 5 s ignition T [°C] Ignition T [°C] Explosion T [°C]	252 (in 0.1 s, no cap used) <sup>[8,14]</sup> 252 (dropping on heated Wood's alloy) <sup>[10,15]</sup> , ~205 <sup>[6]</sup> , 252 <sup>[23]</sup> 205–208 (@ 20 °C/min) <sup>[10]</sup> , 170 (@ 5 °C/min) <sup>[10]</sup> , 206 (@ 20 °C/min, glass tube) <sup>[18]</sup> , 208 (@ 20 °C/min, glass tube) <sup>[18]</sup> , 205 (@ 20 °C/min, iron tube) <sup>[18]</sup> , 207 (@ 20 °C/min, iron tube) <sup>[18]</sup> , 200 (iron tube, 40 s) <sup>[18]</sup> , 205 (iron tube, 0 s) <sup>[18]</sup>																
Thermal stability	Dec. on heating >100 °C in solid state <sup>[6]</sup> , no dec. after heating @ 112 °C in 17 cm of Ar after several hours <sup>[22]</sup> , rate of gas evolution @ 150 °C is slow <sup>[22]</sup> , half life = ~11.5 mins for 8 mg sample heated at 171.4 °C in 23 cm Ar <sup>[22]</sup>																

Vapor pressure [atm. @ °C]	0.25 Pa ( $1.9 \times 10^{-3}$ Torr) (saturated vapor pressure over solid @ RT, glass Bourdon pressure gage) <sup>[20]</sup>  Saturated vapor pressure of liquid cyanuric azide at different temperatures <sup>[20]</sup> :																
	<table border="1"> <thead> <tr> <th>T (K)</th> <th><math>P_s</math> (Pa)</th> </tr> </thead> <tbody> <tr> <td>393.15</td> <td><math>669 \pm 71</math></td> </tr> <tr> <td>403.15</td> <td><math>932 \pm 91</math></td> </tr> <tr> <td>413.15</td> <td><math>1,337 \pm 140</math></td> </tr> <tr> <td>423.15</td> <td><math>1,996 \pm 200</math></td> </tr> <tr> <td>433.15</td> <td><math>2,928 \pm 310</math></td> </tr> <tr> <td>443.15</td> <td><math>5,198 \pm 660</math></td> </tr> <tr> <td>453.15</td> <td><math>7,863 \pm 930</math></td> </tr> </tbody> </table>	T (K)	$P_s$ (Pa)	393.15	$669 \pm 71$	403.15	$932 \pm 91$	413.15	$1,337 \pm 140$	423.15	$1,996 \pm 200$	433.15	$2,928 \pm 310$	443.15	$5,198 \pm 660$	453.15	$7,863 \pm 930$
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443.15	$5,198 \pm 660$																
453.15	$7,863 \pm 930$																
Volatility	Slightly volatile <sup>[18]</sup> , moderately volatile <sup>[19]</sup> , volatile and begins sublimation @ 30 °C <sup>[6]</sup> , highly volatile, saturated vapor pressure is higher than that of NG @ RT <sup>[20]</sup>																
Burn rate [mm/s]	~6 cm/s <sup>[23]</sup>																
Solubility [g/mL]	Insoluble in H <sub>2</sub> O <sup>[8]</sup> , readily soluble in hot EtOH, acetone, benzene and Et <sub>2</sub> O <sup>[8]</sup> , molten cyanuric azide dissolves TNT and other aromatic nitro compounds <sup>[18]</sup>																
Hygroscopicity	Slightly hygroscopic <sup>[18,19]</sup>																
Photosensitivity	LT photolysis of crystals produces triplet nitrene <sup>[17]</sup> , quintet nitrene produced in photolysis @ 4 K <sup>[17]</sup> , septet nitrene formed during photolysis in solid nitrogen matrices <sup>[17]</sup>																
Compatibility	Quick hydrolysis in 0.1 M aq. NaOH solns. @ 50 °C <sup>[17]</sup> , reduced by gaseous H <sub>2</sub> S <sup>[17]</sup> , quantitative reaction with gaseous NH <sub>3</sub> <sup>[17]</sup> , azido groups react with Grignard reagents <sup>[17]</sup> , compatible with Al, stainless steel, RDX, HMX and with some energetic nitramines (DSC) <sup>[6]</sup> , dec. with hot water <sup>[6]</sup>																
Dead pressing	Loses its initiation ability in no. 8 blasting cap on being compressed >20 MPa <sup>[6]</sup>																
Heat of evaporation, $Q_e$ [kJ/mol]	$61.1 \pm 3.3$ (measured) <sup>[20]</sup>																
Heat of melting, $Q_m$ [kJ/mol]	$22.2 \pm 1.3$ (DSC @ 2 K/min, Ar purge, 1.3–3.1 mg sample) <sup>[20]</sup>																
Heat of sublimation, $Q_s$ [kJ/mol]	$83.3 \pm 3.3$ <sup>[20]</sup>																

	Cyanuric azide <sup>[11]</sup>	Cyanuric azide <sup>[12]</sup>
Chemical formula	C <sub>3</sub> N <sub>12</sub>	C <sub>3</sub> N <sub>12</sub>
Molecular weight [g mol <sup>-1</sup> ]	204.12	204.12
Crystal system	Hexagonal	Hexagonal
Space group	P 6 <sub>3</sub>	P-3
a [Å]	8.73	8.7456(2)
b [Å]	8.73	8.7456(2)
c [Å]	5.96	5.8945(3)
α [°]	90	90
β [°]	90	90
γ [°]	120	120
V [Å <sup>3</sup> ]	393.374	390.44(2)
Z	2	2
ρ <sub>calc</sub> [g cm <sup>-3</sup> ]	1.72323	1.736
T [K]	295	183

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- [14] 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**.
- [15] B. T. Fedoroff, O. E. Sheffield, *Encyclopedia of Explosives and Related Items*, vol. 7, US Army Research and Development Command, TACOM, Picatinny Arsenal, USA, **1975**.
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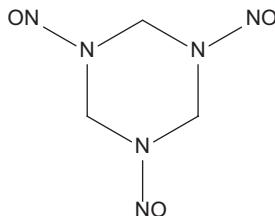
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## Cyclotrimethylene trinitrosamine

Name [German, acronym]: Cyclotrimethylene trinitrosamine, hexahydro-1,3,5-trinitroso-2-triazine, trinitrosotrimethylenetriamine, 1,3,5-trinitroso-1,3,5-triazacyclohexane, 1,3,5-trinitrosohexahydro-s-triazine, 1,3,5-trinitroso-1,3,5-triazinane, hexahydro-1,3,5-trinitroso-1,3,5-triazine [cyclotrimethylentrinitrosamin, TMTA, R-salt, TMTN, R-salz, TNX\*]

Main (potential) use: Ingredient of projectile filler<sup>[5]</sup>, (formed as by-product in the environment from the enzymatic decomposition of RDX<sup>[18]</sup>)

Structural formula:



\* TNX is also (more commonly) used in the literature as the abbreviation for trinitroxylene.

	<b>Cyclotrimethylene trinitrosamine</b>
Formula	C <sub>3</sub> H <sub>6</sub> N <sub>6</sub> O <sub>3</sub>
Molecular mass [g mol <sup>-1</sup> ]	174.12
Appearance at RT	Yellow crystals <sup>[14,17]</sup> , light yellow powder (from citric acid process) <sup>[18]</sup>
IS [J]	8.47–9.97 (15–22 in, 2 kg mass, 17–20 mg sample, P.A.) <sup>[5]</sup> , 0% deton. @ 20 cm (5 kg mass) but 100% deton. @ 50 cm (5 kg mass) <sup>[7]</sup> , H <sub>50%</sub> = 1.25 m (10 kg mass, Bourges capsule, 25–30 mg sample) <sup>[9]</sup> , H <sub>32%</sub> = 1.25 m (10 kg mass, Bourges capsule, 18 mg sample) <sup>[9]</sup> , 50% go @ 25 J cf. 50% go @ 6 J for RDX (5 kg mass, BAM) <sup>[18]</sup>
FS [N]	Unaffected by steel shoe (friction pendulum test) <sup>[5]</sup> , unaffected by fiber shoe (friction pendulum test) <sup>[5]</sup> , >360 (BAM) <sup>[18]</sup>
N [%]	48.27
Ω(CO <sub>2</sub> ) [%]	-55.1
T <sub>phase transition</sub> [°C]	95 (endo, DSC @ 5 K/min, gold pan, either phase transition or loss of water) <sup>[18]</sup>

$T_{\text{m.p.}}$ [°C]	105–106 <sup>[1]</sup> , 105–107 <sup>[5,7]</sup> , 105 (melting begins, molten metal bath, 5 °C/min) <sup>[9]</sup> , 104–106 (freezing point) <sup>[15]</sup> , 106–107 (crude product) <sup>[5]</sup> , 105–107 (recryst. from isoamyl alcohol) <sup>[5]</sup>																		
$T_{\text{dec.}}$ [°C]	150 (onset), 170 (entire) (heated bath @ 5 °C/min) <sup>[5]</sup> , 150 (dec. begins), 170 (dec. complete) (molten metal bath @ 5 °C/min) <sup>[9]</sup> , 105 <sup>[17]</sup> , 150.5 (exo, onset, DSC @ 5 K/min, gold pan) <sup>[18]</sup>																		
$\rho$ [g cm <sup>-3</sup> ]	$1.91 \pm 0.1$ (@ 293.15 K) <sup>[2]</sup> , 1.508 <sup>[3]</sup> , 0.84 g/cc (packing) <sup>[9]</sup> , sp. gr. = 1.508 <sup>[7]</sup> , 1.53 <sup>[17]</sup> $\rho$ under pressure <sup>[9]</sup> :																		
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Heat of formation	392.4 kcal/kg (enthalpy of form.) <sup>[3]</sup> , 1,641.7 kJ/kg (enthalpy of form.) <sup>[3]</sup> , -417.4 kcal/kg <sup>[16]</sup> , -914 cal/g <sup>[5]</sup> , -91.4 cal/g <sup>[9]</sup> , 285.9 ± 2.3 kJ/mol ( $\Delta_f H^\circ$ , (c)) <sup>[19]</sup>																		
Heat of combustion	3,158 cal/g <sup>[5]</sup> , 3,200 kcal/kg (@ C) <sup>[16]</sup>																		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.																
$-\Delta_{\text{ex}} U^\circ$ [kJ kg <sup>-1</sup> ]	5,154	1,148 cal/g <sup>[12]</sup>	850 kcal/g (@ 1.57 g cm <sup>-3</sup> , if detonated by 2.5 g MF) <sup>[7]</sup> 876 cal/g ( $Q_e V$ ) <sup>[5,9]</sup> 900 kcal/kg <sup>[17]</sup> 4,525 [H <sub>2</sub> O (l)] <sup>[3]</sup> 4,397 [H <sub>2</sub> O (g)] <sup>[3]</sup> 3,665 <sup>[5]</sup>																
$T_{\text{ex}}$ [K]	3,435																		
$p_{\text{CJ}}$ [GPa]	23.9	248 (@ 1.57 g cm <sup>-3</sup> , calcd., empirical, Xiong method) <sup>[12]</sup>																	

VoD [ $\text{m s}^{-1}$ ]	7,935 (@ 1.586 $\text{g cm}^{-3}$ , $\Delta_f H = 278.88 \text{ kJ mol}^{-1}$ )	7,890 (@ 1.58 $\text{g cm}^{-3}$ (TMD), calcd., empirical, R-P method) <sup>[11]</sup>	7,300 (@ 1.49 $\text{g cm}^{-3}$ , confined) <sup>[3]</sup>																								
	7,970 (@ 1.58 $\text{g cm}^{-3}$ (TMD), calcd., Aizenshtadt method) <sup>[11]</sup>	7,610 (@ 1.58 $\text{g cm}^{-3}$ (TMD), calcd., K-J method) <sup>[11]</sup>	7,800 (@ 1.57 $\text{g cm}^{-3}$ ) <sup>[4]</sup>																								
	7,777 (@ 1.57 $\text{g cm}^{-3}$ , calcd., empirical, Xiong method) <sup>[12]</sup>		7,000–7,300 (@ 1.42 $\text{g cm}^{-3}$ , 1.2 in charge diameter, cast, no confinement) <sup>[5]</sup>																								
			VoD (paper cartridge confinement, pressed, 1.18 in charge diameter) <sup>[5]</sup> :																								
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$V_0 [\text{L kg}^{-1}]$	844		996 <sup>[3,6]</sup>																								
			853 <sup>[17]</sup>																								

Trauzl test [cm <sup>3</sup> , % TNT]	122–126% TNT <sup>[8]</sup> , 125.5% PA <sup>[7]</sup>																								
Sand test [g]	59.2 g (200 g bomb) <sup>[5]</sup> , 54.1 g (200 g bomb) <sup>[5]</sup>																								
Ballistic mortar test	130% TNT <sup>[5]</sup> , 134% TNT <sup>[8]</sup>																								
Initiating efficiency	0.200 g MF minimum detonating charge <sup>[5]</sup> , 0.100 g LA minimum detonating charge <sup>[5]</sup>																								
5 s explosion T [°C] Deflagration T [°C]	220 <sup>[5]</sup> 300 <sup>[7]</sup>																								
100 °C heat test [% mass loss]	8.79% mass loss in first 48 h @ 100 °C <sup>[5]</sup> , 2.98% mass loss in second 48 h @ 100 °C <sup>[5]</sup> , no explosion in 100 h @ 100 °C <sup>[5]</sup>																								
Vacuum stability test [cm <sup>3</sup> /h]	0.20 cc/40 h @ 90 °C <sup>[5]</sup> , 9.19 cc/40 h @ 100 °C <sup>[5]</sup> , 3.71 cc/40 h @ 100 °C (average value of 5 g sample twice recryst. from isoamyl alcohol) <sup>[5]</sup>																								
Thermal stability	<p>Long-term stability (R-salt loosely packed in covered wooden boxes for 6 years @ ambient temperature but protected from the sun)<sup>[5]</sup>: no color change, mpt. before storage = 104.5 °C, mpt. after storage = 104 °C, no color to iodine starch paper in 15 min in Abel test @ 110 °C<sup>[5]</sup></p> <p>High-temperature dec. (0.02 g in 10 mL test tube, immersed for 10 min in bath heated @ 5 °C/min)<sup>[5]</sup>:</p> <table border="1"> <thead> <tr> <th>Observation</th> <th>T (°C)</th> <th>Observation</th> <th>T (°C)</th> </tr> </thead> <tbody> <tr> <td>Melting begins</td> <td>105</td> <td>Some bubbles</td> <td>110</td> </tr> <tr> <td>Dec. begins</td> <td>150</td> <td>Very slow dec.</td> <td>150</td> </tr> <tr> <td>Nitrous gas</td> <td>160</td> <td>Dec. in 2 min</td> <td>200</td> </tr> <tr> <td>Complete dec.</td> <td>170</td> <td>Dec. in 40 s</td> <td>250</td> </tr> <tr> <td></td> <td></td> <td>Immediate dec.</td> <td>300</td> </tr> </tbody> </table>	Observation	T (°C)	Observation	T (°C)	Melting begins	105	Some bubbles	110	Dec. begins	150	Very slow dec.	150	Nitrous gas	160	Dec. in 2 min	200	Complete dec.	170	Dec. in 40 s	250			Immediate dec.	300
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		Immediate dec.	300																						
Solubility [g/mL]	33.4 g/100 g acetone @ 15 °C <sup>[17]</sup> , 2.35 g/100 g MeOH @ 15 °C <sup>[17]</sup> , 5.3 g/100 g acetic acid @ 15 °C <sup>[17]</sup>																								
Hygroscopicity	0.02% @ 30 °C @ 90% RH <sup>[5]</sup>																								
Photosensitivity	Very light sensitive (particularly UV) <sup>[17]</sup>																								
Compatibility	Easily dec. by acid or alkali or boiling H <sub>2</sub> O <sup>[5,14]</sup> , slight reaction with Fe powder <sup>[5]</sup> , slight reaction with Cu powder <sup>[5]</sup> , slight reaction with Al powder <sup>[5]</sup> , two parts PA and one part R-salt give a violent dec. after 2 h @ 10 °C <sup>[5]</sup> , two parts PA and one part R-salt gives a violent dec. after 10–15 min @ 100 °C <sup>[5]</sup> , dec. by mineral acids even if cold <sup>[17]</sup> , no dec. with pure acetic acid up to 100 °C <sup>[17]</sup>																								
Brisance	4.7 mm <sup>[17]</sup>																								
Fugacity	386 cc <sup>[17]</sup>																								
ΔH <sub>dec</sub> [J/g]	3267 (released, DSC @ 5 K/min, gold pan) <sup>[18]</sup>																								

	Cyclotrimethylene trinitrosamine <sup>[10]</sup>	Cyclotrimethylene trinitrosamine <sup>[13]</sup>	Cyclotrimethylene trinitrosamine <sup>†[13]</sup>	Cyclotrimethylene trinitrosamine <sup>[18]</sup>
Chemical formula	$\text{C}_3\text{H}_6\text{N}_6\text{O}_3$	$\text{C}_3\text{H}_6\text{N}_6\text{O}_3$	$\text{C}_3\text{H}_6\text{N}_6\text{O}_3$	$\text{C}_3\text{H}_6\text{N}_6\text{O}_3$
Molecular weight [g mol <sup>-1</sup> ]	174.12	174.12	174.12	174.12
Crystal system	Monoclinic	Monoclinic	Trigonal	Monoclinic
Space group	not given	<i>P</i> 2 <sub>1</sub> / <i>c</i>	<i>R</i> -3	<i>P</i> 2 <sub>1</sub> / <i>c</i> (no. 14)
<i>a</i> [\AA]	12.83	9.060(1)	36.340	9.0671(6)
<i>b</i> [\AA]	6.26	6.236(1)		6.2475(4)
<i>c</i> [\AA]	9.08	12.874(2)		12.8616(10)
$\alpha$ [°]	90	90		90
$\beta$ [°]	92.55	92.47(1)		
$\gamma$ [°]	90	90	120	90
<i>V</i> [\AA <sup>3</sup> ]	728.545			728.05(9)
<i>Z</i>	4			4
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.587	1.573	1.573	1.5884
<i>T</i> [K]	295			297
				Crystals from slow evaporation of CH <sub>3</sub> CN soln. @ RT

† Crystallizes in triclinic system when crystals are grown from CCl<sub>4</sub> or CHCl<sub>3</sub>.

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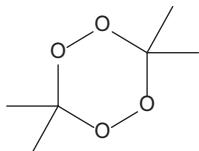
# D

## DADP

Name [German, acronym]: Diacetone diperoxide, 3,3,6,6-tetramethyl-1,2,4,5-tetroxane [DADP]

Main (potential) use: Improvised explosive, suggested as substitute for mercury fulminate in igniters and detonators but has not achieved widespread use due to its low stability

Structural formula:



	DADP
Formula	C <sub>6</sub> H <sub>12</sub> O <sub>4</sub>
Molecular mass [g mol <sup>-1</sup> ]	148.16
Appearance at room temperature (RT)	Colorless crystals
IS [J]	5 (<100 µm), 1.4 <sup>[2]</sup> , 7 cm (2 kg hammer) <sup>[6]</sup> , H <sub>50</sub> = 21.2 ± 1.5 cm (200 g mass, 12 mg pressed sample, Russian K-44-1 impact machine) <sup>[6]</sup> , E <sub>50</sub> = 0.42 (200 g mass, 12 mg pressed sample, Russian K-44-1 impact machine) <sup>[6]</sup> , 13.4 ± 1.8 cm (crude) <sup>[7]</sup> , 18.4 ± 2.9 cm (from fast reaction) <sup>[7]</sup> , 21.0 ± 6.9 cm (from slow reaction) <sup>[7]</sup>
FS [N]	5 (<100 µm), 1.75 <sup>[1]</sup> , 2.99 <sup>[2]</sup> , 2 (50% probability analysis) <sup>[6]</sup> , 49 ± 13 (crude) <sup>[7]</sup> , 19.5 ± 12.3 (from fast reaction) <sup>[7]</sup> , 18.4 ± 5.8 (from slow reaction) <sup>[7]</sup>
ESD [J]	0.2 (<100 µm), 0.026 <sup>[2]</sup> , 26 mJ <sup>[6]</sup> , 0.003 (crude) <sup>[7]</sup> , 0.025 (from fast reaction) <sup>[7]</sup> , 0.063 (from slow reaction) <sup>[7]</sup>
N [%]	0
Ω(CO <sub>2</sub> ) [%]	-151.2
T <sub>m.p.</sub> [°C]	132–133 <sup>[6]</sup> , 130–132 <sup>[6]</sup> , 131–133 <sup>[7]</sup> , 128 <sup>[9]</sup> , ~ 132 (DSC) <sup>[9]</sup> , 132–133 (cryst., sealed capillary tube @ 3 °C/min, Boitus mpt. apparatus) <sup>[10]</sup> , 104.9 (onset of sublimation endo), 125.4 (melting peak max, endo) (DSC @ 10 K/min, Al pans with pierced lid, N <sub>2</sub> ) <sup>[11]</sup>
T <sub>dec.</sub> [°C]	165 <sup>[2,9]</sup>

$\rho$ [g cm <sup>-3</sup> ]	1.33 (@ 208 K) <sup>[1]</sup> , 1.31 (calcd. @ 298 K), 1.331 (crystalline) <sup>[2,9]</sup> , 1.33 (X-ray) <sup>[6]</sup>										
Heat of formation	$-355.1 \text{ kJ/mol } (\Delta_f H^\circ)^{[2]}$ , $-81.4 \text{ kcal/mol } (\Delta_f H^\circ \text{ (g), calcd.})^{[9]}$ , $-415.9 \text{ kJ/mol } (\Delta_f H^\circ \text{ (s), calcd.})^{[9]}$ , $-352.1 \text{ kJ/mol } (\Delta_f H^\circ_{298}, \text{exptl.})^{[5]}$ , $-598.5 \pm 39.7 \text{ kJ/mol } (\Delta_f H^\circ_{298}, \text{exptl., semimicro oxygen bomb calorimetry})^{[10]}$ , $-281 \text{ kJ/mol } (\text{enthalpy of form., est. by semiempirical AM1 with allowance for heat of sublimation})^{[10]}$ , $-361.3 \pm 10.0 \text{ kJ/mol } (\text{enthalpy of form., gas phase, calcd. using G4 method using isodesmic and atomization reactions})^{[10]}$ , $-431.6 \pm 51 \text{ kJ/mol } (\Delta_f H^\circ_{298})^{[10]}$ , $-355.1 \pm 51 \text{ kJ/mol } (\Delta_f H^\circ_{298} \text{ (g)})^{[10]}$ , $-598.5 \pm 39.7 \text{ kJ/mol } (\Delta_f H^\circ)^{[11]}$										
Heat of combustion	$1,985 \text{ kJ/kg}$ (calcd.) <sup>[5]</sup> , 1,985 (heat of combustion under N <sub>2</sub> atmosphere, calcd. from max combustion temperature) <sup>[10]</sup> , $\Delta_c U = -3,642 \pm 51 \text{ kJ/mol}$ (bomb calorimeter) <sup>[10]</sup> , $\Delta_c H = -3,644.5 \pm 51 \text{ kJ/mol}$ <sup>[10]</sup> <p>Measured <math>\Delta_c U^\circ</math> and calculated <math>\Delta H^\circ</math> values from ref.<sup>[11]</sup>:</p> <table border="1"> <thead> <tr> <th colspan="2"><math>\Delta_c U^\circ</math></th> <th><math>\Delta H_c^\circ</math> (kJ/mol)</th> </tr> <tr> <th>J/g</th> <th>kJ/mol</th> <th></th> </tr> </thead> <tbody> <tr> <td><math>-23,456 \pm 268</math></td> <td><math>-3,475.0 \pm 39.7</math></td> <td><math>-3,477.5 \pm 39.7</math></td> </tr> </tbody> </table>	$\Delta_c U^\circ$		$\Delta H_c^\circ$ (kJ/mol)	J/g	kJ/mol		$-23,456 \pm 268$	$-3,475.0 \pm 39.7$	$-3,477.5 \pm 39.7$	
$\Delta_c U^\circ$		$\Delta H_c^\circ$ (kJ/mol)									
J/g	kJ/mol										
$-23,456 \pm 268$	$-3,475.0 \pm 39.7$	$-3,477.5 \pm 39.7$									
	Calcd. (EXPLO5 6.03)	Exptl.									
$-\Delta_{\text{ex}} U^\circ$ [kJ kg <sup>-1</sup> ]	3,194	$2,837^{[2]}$ 2,837 (heat of explosion @ load density = 0.59 g cm <sup>-3</sup> , 1.69 g sample, Al shell, bomb calorimeter) <sup>[10]</sup>									
$T_{\text{ex}}$ [K]	2,032										
$p_{\text{CJ}}$ [kbar]	131										
VoD [m s <sup>-1</sup> ]	6,246	$-^{[2]}$									
$V_0$ [L kg <sup>-1</sup> ]	815	$713^{[2]}$ 713 (@ load density = 0.59 g cm <sup>-3</sup> , 1.69 g sample, Al shell, bomb calorimeter) <sup>[10]</sup>									

Sand test [g]	30.1 g sand crushed (63% TNT) <sup>[6]</sup>														
Initiation efficiency	0.5 g unable to induce detonation of RDX <sup>[6]</sup>														
Thermal stability	Slowly decomposes in solution on heating <sup>[6]</sup>														
Vapor pressure [atm @ °C]	17.7 Pa @ 25 °C (gas chromatography) <sup>[6]</sup> , more volatile than TATP <sup>[11]</sup>														
Heat of sublimation [kJ/mol]	81.9 (Clapeyron eq.) <sup>[6]</sup> , 71.3 (Egorshev eq.) <sup>[6]</sup> , $\Delta H_{\text{sub}} = 18.0 \text{ kcal/mol}$ <sup>[9]</sup> , 76.5 (enthalpy of sublimation) <sup>[10]</sup>														
Heat of evaporation [kJ/mol]	46.5 (Egorshev eq.) <sup>[6]</sup>														
Heat of melting [kJ/mol]	24.7 (Egorshev eq.) <sup>[6]</sup> , 140 J/g (DSC) <sup>[9]</sup>														
Burn rate [mm/s]	Dependence of the burn rate on pressure <sup>[6]</sup> : <table border="1"> <thead> <tr> <th>Pressure (MPa)</th> <th>Burn rate (mm s<sup>-1</sup>)</th> </tr> </thead> <tbody> <tr> <td>0.05</td> <td>~ 1.2</td> </tr> <tr> <td>0.1</td> <td>~ 2</td> </tr> <tr> <td>0.2</td> <td>~ 3.4</td> </tr> <tr> <td>0.5</td> <td>~ 8</td> </tr> <tr> <td>1</td> <td>~ 13</td> </tr> <tr> <td>2</td> <td>~ 28</td> </tr> </tbody> </table>	Pressure (MPa)	Burn rate (mm s <sup>-1</sup> )	0.05	~ 1.2	0.1	~ 2	0.2	~ 3.4	0.5	~ 8	1	~ 13	2	~ 28
Pressure (MPa)	Burn rate (mm s <sup>-1</sup> )														
0.05	~ 1.2														
0.1	~ 2														
0.2	~ 3.4														
0.5	~ 8														
1	~ 13														
2	~ 28														
Solubility [g/mL]	Practically insoluble in H <sub>2</sub> O <sup>[6]</sup> , soluble in most common organic solvents <sup>[6]</sup> , purification by recryst. from hot methanol <sup>[7]</sup> , recryst. from acetone <sup>[7]</sup> , recryst. from hot ethanol <sup>[10]</sup>														
DDT	Transition distance = 4.7 mm, 25% TMD (DADP from slow reaction) <sup>[7]</sup>														
Heat of dec. [J/g]	76 (DSC) <sup>[9]</sup>														
Max. combustion T [K]	1,125 <sup>[10]</sup>														

	DADP <sup>[3]</sup>	DADP <sup>[4]</sup>	DADP <sup>[7]</sup>	DADP <sup>[8]</sup>	DADP <sup>[7]</sup>
Chemical formula	C <sub>6</sub> H <sub>12</sub> O <sub>4</sub>	C <sub>6</sub> H <sub>12</sub> O <sub>4</sub> /C <sub>12</sub> H <sub>24</sub> O <sub>8</sub>	C <sub>6</sub> H <sub>12</sub> O <sub>4</sub>	C <sub>6</sub> H <sub>12</sub> O <sub>4</sub>	C <sub>6</sub> H <sub>12</sub> O <sub>4</sub>
Molecular weight [g mol <sup>-1</sup> ]	148.16	148.16/296.31	148.16	148.16	148.16
Crystal system	Monoclinic	Monoclinic		Monoclinic	
Space group	P 2/c (no. 13)	P 2/c (no. 13)		P 2/c (no. 13)	
<i>a</i> [Å]	5.9152(18)	5.8881(8)	5.86(4)	5.9194(8)	5.86(4)

<i>b</i> [Å]	5.9221(18)	5.8935(8)	5.87(3)	5.9245(8)	5.88(4)
<i>c</i> [Å]	10.585(3)	10.5238(14)	10.43(5)	10.5821(14)	10.55(7)
$\alpha$ [°]	90	90	90	90	90
$\beta$ [°]	94.344(5)	94.380(2)	93.83(15)	94.326(3)	83.03(9)
$\gamma$ [°]	90	90	90	90	90
<i>V</i> [Å <sup>3</sup> ]	369.72(19)	364.13(9)	358(6)	370.05(9)	358(6)
<i>Z</i>	2	1	2	2	2
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.331	1.351	1.372	1.330	1.372
<i>T</i> [K]	203	120	100	208	100
	Crystals obtained from hot methanol, extremely fine crystals	Recryst. by heated acetone/H <sub>2</sub> O <sub>2</sub> to 70 °C with adjusted pH	Recryst. from CH <sub>2</sub> Cl <sub>2</sub> , striated blocks	Recryst. from acetone, fine prisms	Recryst. from MeOH/ acetic acid, small blocks

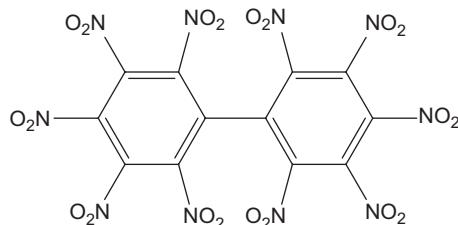
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## Decanitrobiphenyl

Name [German, acronym]: 2,2',3,3',4,4'5,5',6,6'-Decanitrobiphenyl,  
[decanitrobiphenyl, DNBP]

Main (potential) use: Zero-hydrogen nitrocarbon explosive

Structural formula:



	Decanitrobiphenyl		
Formula	$C_{12}N_{10}O_{20}$		
Molecular mass [g mol <sup>-1</sup> ]	604.18		
Appearance at RT	Pale yellow prism crystals <sup>[1]</sup>		
N [%]	23.18		
$\Omega(CO_2)$ [%]	-10.6		
$T_{m.p.}$ [°C]			
$T_{dec.}$ [°C]	243–248 (dec.) <sup>[1]</sup>		
$\rho$ [g cm <sup>-3</sup> ]	1.86 <sup>[2]</sup>		
Heat of formation			
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{ex}U^o$ [kJ kg <sup>-1</sup> ]			
$T_{ex}$ [K]			
$p_{c,l}$ [kbar]		352 (@ 1.95 g cm <sup>-3</sup> , calcd.) <sup>[2]</sup>	
VoD [m s <sup>-1</sup> ]		8,660 (@ 1.95 g cm <sup>-3</sup> , calcd.) <sup>[2]</sup>	
$V_0$ [L kg <sup>-1</sup> ]			

Thermal stability	Slowly dec. in standing over $\text{CaCl}_2$ in a desiccator in the dark @ 25 °C and forms dark, oily solid after 3–4 months <sup>[1]</sup>
Solubility [g/mL]	Much less soluble in common organic solvents than HNB <sup>[1]</sup> , not measurably soluble in boiling $\text{CH}_2\text{Cl}_2$ , benzene or $\text{CHCl}_3$ <sup>[1]</sup> , dissolves in boiling $\text{CH}_3\text{CN}$ or 1,2-dichloroethane with some dec. <sup>[1]</sup>
Compatibility	Reacts rapidly with water or aqueous bases <sup>[1]</sup> , reacts rapidly with ammonia if suspended in benzene <sup>[1]</sup>

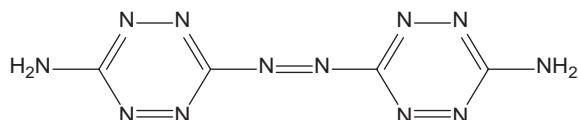
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## Diaminoazobistetrazine

Name [German, acronym]: 3,3'-Azobis(6-amino-1,2,3,5-tetrazine),  
[diaminobistetrazin, DAAT, DAATz]

Main (potential) use: Possible use in rocket propellants and IHE formulations<sup>[1]</sup>

Structural formula:



	DAAT	
Formula	C <sub>4</sub> H <sub>4</sub> N <sub>12</sub>	
Molecular mass [g mol <sup>-1</sup> ]	220.16	
Appearance at RT		
IS [J]	5 <sup>[2]</sup>	
FS [N]	324 <sup>[2]</sup>	
N [%]	76.0	
Ω(CO <sub>2</sub> ) [%]	-72.7	
T <sub>m.p.</sub> [°C]		
T <sub>dec.</sub> [°C]		
ρ [g cm <sup>-3</sup> ]	1.76 <sup>[2]</sup>	
Heat of formation	1,032 kJ/mol <sup>[1]</sup> , 4.70 kJ/g ( $\Delta_f H^\circ$ ) <sup>[2]</sup>	
Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
-Δ <sub>ex</sub> U <sup>o</sup> [kJ kg <sup>-1</sup> ]		
T <sub>ex</sub> [K]		
p <sub>C,J</sub> [kbar]		
VoD [m s <sup>-1</sup> ]		
V <sub>0</sub> [L kg <sup>-1</sup> ]		

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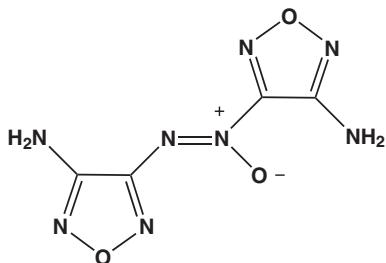
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### 3,3'-Diamino-4,4'-azoxyfurazan

Name [German, acronym]: 3,3'-Diamino-4,4'-azoxyfurazan, diaminoazoxy-furazan  
[DAAF]

Main (potential) use: Secondary (high) explosive

Structural formula:



	<b>DAAF</b>
Formula	C <sub>4</sub> H <sub>4</sub> N <sub>8</sub> O <sub>3</sub>
Molecular mass [g mol <sup>-1</sup> ]	212.13
Appearance at RT	
IS [J]	7, >320 Nm <sup>[4]</sup> , drop height >320 cm (2.5 kg mass, type 12 tool) <sup>[5,16]</sup> , IS <sub>LL</sub> = 1.0 m <sup>[10]</sup> , IS <sub>A50</sub> = 2.2 m <sup>[10]</sup> , >78 <sup>[13]</sup> , H <sub>50</sub> = <320 cm (type 12 DWI apparatus) <sup>[14]</sup> , >50 <sup>[17]</sup> , A <sub>d1</sub> = 20%, A <sub>d2</sub> = 20%, LL = 1.0 m, A <sub>50 d1</sub> = 2.2 m, A <sub>50 d2</sub> = 4.3 <sup>[19]</sup> , H <sub>50</sub> ≥ 320 cm <sup>[20]</sup>
FS [N]	>360 <sup>[4,17]</sup> , >36 kg (BAM) <sup>[5]</sup> , p <sub>fr,LL</sub> = 450 MPa <sup>[10,19]</sup> , p <sub>fr,50%</sub> = 660 MPa <sup>[10,19]</sup> , <360 <sup>[13]</sup> , >36.0 kg <sup>[14,20]</sup> , >353 <sup>[17]</sup>
ESD [J]	0.0625, 0.36 <sup>[5]</sup> , 0.0625 (spark TIL) <sup>[13,14]</sup> , 0 goes out of 13 @ 0.36 J <sup>[20]</sup>
N [%]	52.82
Ω(CO <sub>2</sub> ) [%]	-52.8
T <sub>m,p.</sub> [°C]	Dec. without melting <sup>[6]</sup>
T <sub>dec.</sub> [°C]	229, 249 <sup>[6]</sup> , 248 (onset, DSC) <sup>[7]</sup> , 220 (onset), 260 (peak exotherm, DSC) <sup>[13,14]</sup> , 249 (onset, DSC) <sup>[17]</sup> , 250 (onset, DSC) <sup>[20]</sup>
ρ [g cm <sup>-3</sup> ]	1.745 (@ 298 K), 1.75 <sup>[6]</sup> , 1.764 (crystal) <sup>[6]</sup> , 1.70 <sup>[12]</sup> , 1.747 <sup>[13,14]</sup> , 1.747 (crystal) <sup>[16,17]</sup>

	DAAF produced using different routes, values from ref. <sup>[15]</sup> :		
	Material	$\rho_{av}$ (g cm <sup>-3</sup> )	Particle size (μm)
	ATK produced DAAF pressed to high density	1.685	80
	DAAF prepared using LANL process, pressed to high density	1.688	40
	ATK produced DAAF but crash precipitated in DMSO	1.592	<5
	ATK produced DAAF, low density	1.596	80
	DAAF prepared using LANL process, low density	1.597	40
Heat of formation	443 kJ/mol ( $\Delta_f H^o$ ) <sup>[11]</sup> , 354 kJ/mol ( $\Delta_f H$ ) <sup>[11]</sup> , 106 kcal/mol ( $\Delta_f H$ ), measured by combustion calorimetry) <sup>[7]</sup> , 106 kcal/mol ( $\Delta_f H$ ) <sup>[13,14,16]</sup> , 444 kJ/mol (enthalpy of form.) <sup>[17]</sup> , 443.5 kJ/mol ( $\Delta_f H$ ) <sup>[12]</sup>		
	Calcd. (EXPL05 6.03)	Lit. values	Exptl.
$-\Delta_{ex}U^o$ [kJ kg <sup>-1</sup> ]	5,081	9,263 kJ/dm <sup>3</sup> (volumetric enthalpy of explosion, calcd., CHEETAH 2.0) [H <sub>2</sub> O (l)] <sup>[17]</sup>  9.139 kJ/cm <sup>3</sup> (total energy of detonation @ 0.1 MPa, calcd., CHEETAH 2.0) <sup>[17]</sup>	
$T_{ex}$ [K]	3,589	3,155 (@ 1.747 g cm <sup>-3</sup> , $\Delta H_f = 443.5$ kJ/mol, calcd., JAGUAR) <sup>[18]</sup>	
$p_{CJ}$ [kbar]	275	306 (@ 1.685 g cm <sup>-3</sup> ) <sup>[13,14]</sup>  29.3 GPa (@ 1.747 g cm <sup>-3</sup> , calcd., CHEETAH 2.0) <sup>[17]</sup>  28.2 GPa (@ 1.747 g cm <sup>-3</sup> , $\Delta H_f = 443.5$ kJ/mol, calcd., JAGUAR) <sup>[18]</sup>	306 (@ 1.685 g cm <sup>-3</sup> ) <sup>[4]</sup>  299 (@ 1.69 g cm <sup>-3</sup> , est. from 0.5 in diameter plate dent) <sup>[5]</sup>

VoD [ $\text{m s}^{-1}$ ]	8316	8,240 (@ 1.747 g $\text{cm}^{-3}$ , calcd., CHEETAH 2.0) <sup>[17]</sup> 7,930 (@ 1.685 g $\text{cm}^{-3}$ ) <sup>[13,14]</sup> 8,124 (@ TMD, calcd., CHEETAH v8.0) <sup>[7]</sup> 8,160 (@ 1.747 g $\text{cm}^{-3}$ , $\Delta H_f = 443.5 \text{ kJ/mol}$ , calcd., JAGUAR) <sup>[18]</sup> 7,930 (@ 1.685 g $\text{cm}^{-3}$ , calcd., JAGUAR) <sup>[25]</sup>	7,930 (@ 1.685 g $\text{cm}^{-3}$ ) <sup>[4]</sup> 8,110 ± 30 8,050 (est. LASEM method) <sup>[7]</sup> 8,110 (@ TMD, large-scale detonation) <sup>[7]</sup> 7,930 (@ 1.685 g $\text{cm}^{-3}$ ) <sup>[18]</sup>
$V_0 [\text{L kg}^{-1}]$	758		

Critical diameter [cm]	<3 mm <sup>[13,14]</sup>					
Shock velocity imaging	Pressure required to initiate DAAF as a function of DAAF particle size and $\rho$ <sup>[14]</sup> :					
	Gap thickness (mm)	Pressure (GPa)	Gap thickness (mm)	Pressure (GPa)		
	2.03	8.3	3.03	4.5–4.8		
	2.54	4.83	3.30	4.48		
SSGT [cm]	DAAF produced using different routes (Bruceton up/down method), shock sensitivity values from LANL SSGT <sup>[15]</sup> :					
	Material	$\rho_{\text{av.}} (\text{g cm}^{-3})$	50% point (mm)			
	DAAF prepared using LANL process (high $\rho$ )	1.69	1.91			
	DAAF prepared using LANL process (low $\rho$ )	1.59	3.12			
	ATK produced DAAF (high $\rho$ )	1.69	2.74			
	ATK produced DAAF (low $\rho$ )		3.35			
	ATK produced DAAF but crash precipitated in DMSO	1.59	3.02			
	1.91 mm ( $\rho = 1.69 \text{ g cm}^{-3}$ , 50% point, LANL SSGT) <sup>[17]</sup>					
Vacuum stability test [ $\text{cm}^3/\text{h}$ ]	0.42 mL/g @ 100 °C <sup>[20]</sup>					
Laser ignition	Ignition delay (s) as a function of laser irradiance ( $\text{W/cm}^2$ ) (approx. values from graph): 0.2 s/100 W/ $\text{cm}^2$ , 0.18 s/125 W/ $\text{cm}^2$ , 0.12 s/140 W/ $\text{cm}^2$ , 0.1 s/150 W/ $\text{cm}^2$ <sup>[20]</sup>					

	DAAF <sup>[8]</sup>	DAAF <sup>[9]</sup>
Chemical formula	C <sub>4</sub> H <sub>4</sub> N <sub>8</sub> O <sub>3</sub>	C <sub>4</sub> H <sub>4</sub> N <sub>8</sub> O <sub>3</sub>
Molecular weight [g mol <sup>-1</sup> ]	212.15	212.15
Crystal system	Monoclinic	Monoclinic
Space group	P 2 <sub>1</sub> /c (no. 14)	P 2 <sub>1</sub> /c (no. 14)
a [Å]	4.6466(6)	9.3212(8)
b [Å]	9.6326(10)	9.6326(9)
c [Å]	9.0243(11)	8.9004(8)
α [°]	90	90
β [°]	91.607(9)	91.3434(19)
γ [°]	90	90
V [Å <sup>3</sup> ]	403.76(8)	798.9(2)
Z	2	4
ρ <sub>calc</sub> [g cm <sup>-3</sup> ]	1.745	1.764
T [K]	294	233

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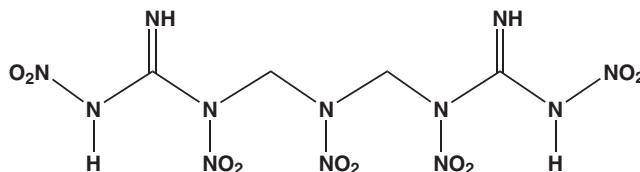
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## 1,7-Diamino-1,7-dinitrimino-2,4,6-trinitro-2,4,6-triazahexane

Name [German, acronym]: 1,7-Diamino-1,7-dinitrimino-2,4,6-trinitro-2,4,6-triazahexane [1,7-diamino-1,7-dinitrimino-2,4,6-trinitro-2,4,6-triazahexane, APX]

Main (potential) use: Primary explosive<sup>[1]</sup>, possible future energetic filler in high explosive formulations<sup>[2]</sup>

Structural formula:



	APX		
Formula	$\text{C}_4\text{H}_8\text{N}_{12}\text{O}_{10}$		
Molecular mass [g mol <sup>-1</sup> ]	384.18		
Appearance at RT	Colorless platelets <sup>[2]</sup>		
IS [J]	$\sim 3^{[1]}, \geq 3$ (<100 $\mu\text{m}$ , BAM) <sup>[2]</sup> , 5 (95% APX with 5 wt.% PVAA, BAM) <sup>[2]</sup>		
FS [N]	$\sim 80^{[1]}, \geq 80$ (<100 $\mu\text{m}$ , BAM) <sup>[2]</sup> , 160 (95% APX with 5 wt.% PVAA, BAM) <sup>[2]</sup>		
ESD [J]	$\sim 0.1^{[1]}, \geq 0.1$ (<100 $\mu\text{m}$ , OZM apparatus) <sup>[2]</sup>		
N [%]	43.75		
$\Omega(\text{CO}_2)$ [%]	-8.33		
$T_{\text{dec.}}$ [ $^{\circ}\text{C}$ ]	174 (exo, onset, DSC @ 5 $^{\circ}\text{C}/\text{min}$ , covered Al containers, hole in lid) <sup>[2]</sup>		
$\rho$ [g cm <sup>-3</sup> ]	1.91 <sup>[1]</sup>		
Heat of formation	272.1 kJ/mol ( $\Delta_f H^\circ$ , (s), calcd., CBS-4M) <sup>[2]</sup> , 805.0 kJ/kg ( $\Delta_f U^\circ$ , (s), calcd., CBS-4M) <sup>[2]</sup>		
Heat of combustion	1,783 cal/g (bomb calorimetry) <sup>[2]</sup>		
	Calcd. (EXPLO5 5.03)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^\circ$ [kJ kg <sup>-1</sup> ]	5,935 <sup>[2]</sup>		
$T_{\text{ex}}$ [K]	4,489 <sup>[2]</sup>		
$p_{\text{C-J}}$ [kbar]	398 <sup>[2]</sup>		

VoD [ $\text{m s}^{-1}$ ]	9,540 (@ 1.911 $\text{g cm}^{-3}$ ) <sup>[2]</sup>	9,650 (@ 1.911 $\text{g cm}^{-3}$ ) <sup>[1]</sup>	4,853 (@ 0.63 $\text{g cm}^{-3}$ , EXPLOMET-FO-2000) <sup>[2]</sup>
$V_0$ [ $\text{L kg}^{-1}$ ]	816 <sup>[2]</sup>		
Thermal stability	No dec. or mass loss in Radex oven @ 75 °C for 48 h <sup>[2]</sup>		
Solubility [g/mL]	Recryst. from $\text{CHCl}_3$ /acetone soln. <sup>[2]</sup>		
$\Delta H_{\text{sub}}$ [kcal/mol]	19.2 <sup>[2]</sup>		
Koenen test	Rupture of steel tube into part powder-like pieces (<100 $\mu\text{m}$ , 19.0 g APX, 10 mm orifice) <sup>[2]</sup>		

APX <sup>[2]</sup>	
Chemical formula	$\text{C}_4\text{H}_8\text{N}_{12}\text{O}_{10}$
Molecular weight [g mol <sup>-1</sup> ]	384.18
Crystal system	Orthorhombic
Space group	<i>Pbcn</i> (no. 60)
<i>a</i> [\mathring{A}]	8.9909(18)
<i>b</i> [\mathring{A}]	6.3392(13)
<i>c</i> [\mathring{A}]	23.4311(47)
$\alpha$ [°]	90
$\beta$ [°]	90
$\gamma$ [°]	90
<i>V</i> [\mathring{A} <sup>3</sup> ]	1,335.5(5)
<i>Z</i>	4
$\rho_{\text{calc}}$ [g $\text{cm}^{-3}$ ]	1.911
<i>T</i> [K]	200
	Colorless platelet crystals from evaporation of $\text{CHCl}_3$ /acetone mixture @ RT

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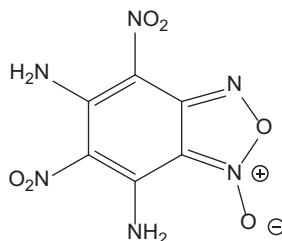
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## 5,7-Diamino-4,6-dinitrobenzofuroxan

Name [German, acronym]: Diamino-dinitrobenzofuroxan [diamino-dinitrobenzofuroxan, DADNBF, CL-14]

Main (potential) use: Possible new insensitive, high-performance explosive<sup>[1]</sup>

Structural formula:



	<b>CL-14</b>
Formula	C <sub>4</sub> H <sub>4</sub> N <sub>6</sub> O <sub>6</sub>
Molecular mass [g mol <sup>-1</sup> ]	256.13
Appearance at RT	Yellow solid or crystals <sup>[3]</sup> , dark yellow solid (crude product) <sup>[10]</sup>
IS [J]	DH <sub>50</sub> = 94 cm <sup>[1]</sup> , 129 cm <sup>[3,4]</sup> , 50% TNT <sup>[5]</sup> , H <sub>50%</sub> = 120 cm (2.5 kg, 35 mg sample, garnet paper, type 12 tool, B.M.) <sup>[6]</sup> , 30 <sup>[7]</sup> , 214.9 cm (CL-14 with 3% Viton A binder, type 12B, 2.5 kg) <sup>[8]</sup> , H <sub>50%</sub> = 120 cm (2.5 kg mass) <sup>[9]</sup>
FS [N]	>36 kg <sup>[1]</sup> , 360 <sup>[7]</sup> , >360 (CL-14 with 3% Viton A binder) <sup>[8]</sup>
ESD [J]	0.0625 (CL-14 with 3% Viton A binder) <sup>[8]</sup>
N [%]	32.81
Ω(CO <sub>2</sub> ) [%]	-25.0
T <sub>m.p.</sub> [°C]	294 <sup>[2]</sup> , 290–291 (dec.) <sup>[10]</sup> , 291 (endo followed by exo, DTA @ 10 °C/min) <sup>[10]</sup> , 289–291 <sup>[10]</sup> , 289 (dec., 95% CL-14, 5% polyurethane (PU)) <sup>[10]</sup> , 288 (dec., 90% CL-14, 10% PU) <sup>[10]</sup> , 288 (dec., 85% CL-14, 15% PU) <sup>[10]</sup>
T <sub>b.p.</sub> [°C]	
T <sub>phase transition</sub> [°C]	
T <sub>dec.</sub> [°C]	228 (onset, CL-14 with 3% Viton A binder, DSC @ 10 °C/min) <sup>[8]</sup> , 290–291 <sup>[10]</sup> , 291 (endo followed by exo, DTA @ 10 °C/min) <sup>[10]</sup> , 289 (dec., 95% CL-14, 5% PU) <sup>[10]</sup> , 288 (dec., 90% CL-14, 10% PU) <sup>[10]</sup> , 288 (dec., 85% CL-14, 15% PU) <sup>[10]</sup> , 291 (DTA, 95% CL-14, 5% PU) <sup>[10]</sup> , 291 (DTA, 90% CL-14, 10% PU) <sup>[10]</sup> , 289 (DTA, 85% CL-14, 15% PU) <sup>[10]</sup> , 289.3 (exo, onset, DSC @ 10 °C/min) <sup>[10]</sup> , 289.1 (exo, onset, DSC @ 10 °C/min, 95% CL-14, 5% PU) <sup>[10]</sup> , 290 (exo, onset, DSC @ 10 °C/min, 90% CL-14, 10% PU) <sup>[10]</sup> , 290 (exo, onset, DSC @ 10 °C/min, 85% CL-14, 15% PU) <sup>[10]</sup>

$\rho$ [g cm <sup>-3</sup> ]	1.91 (crystal) <sup>[1]</sup> , 1.89 (calcd.) <sup>[6]</sup> , 1.95 (obs.) <sup>[6]</sup> , 1.941 (TMD) <sup>[8]</sup> , 1.91 (TMD) <sup>[10]</sup> , 1.91 (exptl.) <sup>[10]</sup> , 1.85 (TMD, 95% CL-14, 5% PU) <sup>[10]</sup> , 1.80 (TMD, 90% CL-14, 10% PU) <sup>[10]</sup> , 1.75 (TMD, 85% CL-14, 15% PU) <sup>[10]</sup> , 1.54 (95% CL-14, 5% PU) <sup>[10]</sup> , 1.49 (TMD, 90% CL-14, 10% PU) <sup>[10]</sup> , 1.44 (TMD, 85% CL-14, 15% PU) <sup>[10]</sup>		
Heat of formation			
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^\circ$ [kJ kg <sup>-1</sup> ]			
$T_{\text{ex}}$ [K]			
$p_{\text{C-J}}$ [kbar]		295 (calcd.) <sup>[3]</sup>  295 (@ 1.89 g cm <sup>-3</sup> , calcd.) <sup>[6]</sup>  26.6 GPa (@ 1.805 g cm <sup>-3</sup> , 93.1% TMD, calcd., Davis eq.) <sup>[8]</sup>  24.7 GPa (@ 1.805 g cm <sup>-3</sup> , 93.1% TMD, calcd., CHEETAH, library exp6.v7.1) <sup>[8]</sup>	
$\text{VoD}$ [m s <sup>-1</sup> ]		8,050 (calcd., $\rho$ not given) <sup>[3,4]</sup>  8,050 (@ 1.89 g cm <sup>-3</sup> , calcd.) <sup>[6]</sup>  7,716 (@ 1.805 g cm <sup>-3</sup> , 93.1% TMD, calcd., CHEETAH, library exp6. v7.1) <sup>[8]</sup>	8,220 ( $\rho$ not given) <sup>[3,4]</sup>  7,720 ± 6 (@ 1.805 g cm <sup>-3</sup> , 93.1% TMD) <sup>[8]</sup>
$V_0$ [L kg <sup>-1</sup> ]			
Critical diameter [cm]	Failure diameter <math>\frac{d}{2}</math> in based on plate dent test <sup>[3]</sup>		
Deflagration $T$ [°C]	290 <sup>[10]</sup> , 290 (95% CL-14, 5% PU) <sup>[10]</sup> , 292 (90% CL-14, 10% PU) <sup>[10]</sup> , 290 (85% CL-14, 15% PU) <sup>[10]</sup>		

Vacuum stability test [cm <sup>3</sup> /h]	0.24 mL gas evolved after 48 h @ 120 °C (CL-14 with 3% Viton A binder) <sup>[8]</sup> , 0.30 cc/5 g/120 °C/40 h <sup>[10]</sup> , 0.53 cc/5 g/120 °C/40 h (95% CL-14, 5% PU) <sup>[10]</sup> , 0.61 cc/5 g/120 °C/40 h (90% CL-14, 10% PU) <sup>[10]</sup> , 0.87 cc/5 g/120 °C/40 h (85% CL-14, 15% PU) <sup>[10]</sup>
Solubility [g/mL]	Soluble in DMSO <sup>[2]</sup> , lower solubility in acetone, nitromethane and acetonitrile <sup>[3]</sup> , recryst. from DMF <sup>[10]</sup>
Compatibility	Compatible with ethylene-vinyl acetate copolymer (EVA) <sup>[3]</sup> , good thermal stability in PBX using PU as binder <sup>[10]</sup>
Plate dent test	Plate dent = 0.085 in, 67.5% of standard (CL-14/EVA, 91/9) and 91.4% of RDX (two 1 in long by ½ in diameter cylinders stacked on a 1 in thick witness plate. A ½ in × ½ in cylinder of PBXN-5 (booster) and RP-80 detonator (to initiate explosive train) were placed on top of each stack) <sup>[3,4]</sup>
Compression strength [kg/cm <sup>2</sup> ]	217.0 (95% CL-14, 5% PU) <sup>[10]</sup> , 134.7 (90% CL-14, 10% PU) <sup>[10]</sup> , 101.1 (85% CL-14, 15% PU) <sup>[10]</sup>

Recryst. of powder CL-14 under vacuum from DMF forms large, cube-like crystals<sup>[3]</sup>, and recryst. from soln. at high temperature followed by slow cooling produces fine crystals<sup>[3]</sup>. Recryst. by extraction at the appropriate temperature can be performed using acetonitrile, dimethylformamide, acetone, nitromethane or *N*-methylpyrrolidinone as the solvent<sup>[3]</sup>. Dimethylformamide, acetone and *N*-methylpyrrolidinone produce cube-like crystals<sup>[3]</sup>. The largest crystals resulted from the use of reagent-grade dimethylformamide<sup>[3,4]</sup>. CL-14 recrystallization by extraction; <sup>a</sup> Malvern Instruments Easy Particle Sizer, M3.0, <sup>b</sup>optical microscope, <sup>c</sup>reagent grade used directly from the bottle, <sup>d</sup>a small amount of rubbery polymeric material separated with the CL-14<sup>[3,4]</sup>:

Solvent	T/pressure	Average particle size, µm <sup>a</sup>	Particle shape <sup>b</sup>
Acetonitrile	79 °C/atm	24.9	Needles ~ 6:1
DMF <sup>c</sup>	103 °C/155 mm	50.4	Cube-like
Acetone	55 °C/atm	10.7	Cube-like
Nitromethane	99 °C/atm	11.5	Needles
<i>N</i> -Methylpyrrolidinone	107 °C/32 mm	26.8	Cube-like <sup>d</sup>

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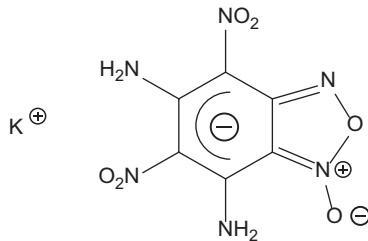
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## 5,7-Diamino-4,6-dinitrobenzofuroxan, potassium salt

Name [German, acronym]: Potassium salt of CL-14, [kalium 5,7-diamino-4,6-dinitrobenzofuroxan, K CL-14]

Main (potential) use: unknown

### Structural formula:



$V_0$ [L kg <sup>-1</sup> ]			
5 s explosion $T$ [°C]	264 (bang) <sup>[1]</sup>		

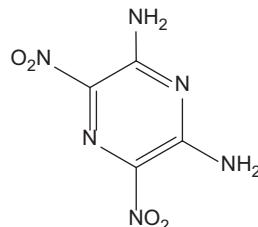
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## 2,6-Diamino-3,5-dinitro-1,4-pyrazine

Name [German, acronym]: 2,6-Diamino-3,5-dinitropyrazine, [2,6-diamino-3,5-dinitropyrazin, ANPZ]

Main (potential) use: Precursor to LLM-105<sup>[4]</sup>

Structural formula:



	ANPZ		
Formula	C <sub>4</sub> H <sub>4</sub> N <sub>6</sub> O <sub>4</sub>		
Molecular mass [g mol <sup>-1</sup> ]	200.13		
Appearance at RT	Yellow plates <sup>[2]</sup> , bright yellow crystalline material <sup>[3]</sup> , yellow powder <sup>[3,4]</sup>		
IS [J]	Insensitivity is so large that it cannot be accurately measured <sup>[2]</sup> , less sensitive than ANPZO (>117 cm) <sup>[2]</sup> , >177 cm <sup>[4]</sup>		
FS [N]	°/₁₀ @ 36.0 kg <sup>[4]</sup>		
ESD [J]	°/₁₀ @ 1.0 J @ 510 Ω <sup>[4]</sup>		
N [%]	42.00		
Ω(CO <sub>2</sub> ) [%]	-48.0		
T <sub>m.p.</sub> [°C]	Dec. before melting @ T>300 <sup>[1]</sup>		
T <sub>dec.</sub> [°C]	Dec. before melting @ T>300 <sup>[1]</sup> , 300 (yellow crystals changes to dark, sealed tube), 356 (darkened yellow crystals dec. with gas evolution) <sup>[3]</sup> , 356 (peak, DSC) <sup>[4]</sup>		
ρ [g cm <sup>-3</sup> ]	1.840 <sup>[4]</sup> , 1.700 @ RT (92.4% TMD) <sup>[4]</sup>		
Heat of formation			
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
-Δ <sub>ex</sub> U° [kJ kg <sup>-1</sup> ]			
T <sub>ex</sub> [K]			
p <sub>c,j</sub> [kbar]			

VoD [ $\text{m s}^{-1}$ ]																																			
$V_0$ [ $\text{L kg}^{-1}$ ]																																			
5 s explosion $T$ [ $^\circ\text{C}$ ] Explosion $T$ [ $^\circ\text{C}$ ]	<p>214.7 <math>^\circ\text{C} &gt; T_{\text{li}} &gt; 192.0 \text{ }^\circ\text{C}</math> (ODTX data, lowest <math>T</math> @ which explosion would occur)<sup>[4]</sup>            ODTX data<sup>[4]</sup>:</p> <table border="1"> <thead> <tr> <th><math>T</math> (<math>^\circ\text{C}</math>)</th> <th>Time to explosion (s)</th> <th><math>T</math> (<math>^\circ\text{C}</math>)</th> <th>Time to explosion (s)</th> </tr> </thead> <tbody> <tr> <td>333.8</td> <td>61</td> <td>253.2</td> <td>1,294</td> </tr> <tr> <td>314.1</td> <td>147</td> <td>253.2</td> <td>1,283</td> </tr> <tr> <td>314.1</td> <td>157</td> <td>239.7</td> <td>4,120</td> </tr> <tr> <td>298.3</td> <td>170</td> <td>226.9</td> <td>12,387</td> </tr> <tr> <td>282.4</td> <td>245</td> <td>214.7</td> <td>34,425</td> </tr> <tr> <td>282.4</td> <td>247</td> <td>192.0</td> <td>167,826 (46.6. h) (no thermal explosion)</td> </tr> <tr> <td>267.4</td> <td>503</td> <td></td> <td></td> </tr> </tbody> </table>			$T$ ( $^\circ\text{C}$ )	Time to explosion (s)	$T$ ( $^\circ\text{C}$ )	Time to explosion (s)	333.8	61	253.2	1,294	314.1	147	253.2	1,283	314.1	157	239.7	4,120	298.3	170	226.9	12,387	282.4	245	214.7	34,425	282.4	247	192.0	167,826 (46.6. h) (no thermal explosion)	267.4	503		
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267.4	503																																		
Solubility [g/mL]	Insoluble in most common organic solvents <sup>[1]</sup> , soluble in 1:1 DMSO/water <sup>[3]</sup> ,																																		
CRT @ 120 °C	0.03 cc/g <sup>[4]</sup>																																		

	ANPZ <sup>[1]</sup>	ANPZ <sup>[2]</sup>
Chemical formula	$\text{C}_4\text{H}_4\text{N}_6\text{O}_4$	$\text{C}_4\text{H}_4\text{N}_6\text{O}_4$
Molecular weight [ $\text{g mol}^{-1}$ ]	200.13	200.13
Crystal system	Monoclinic	Monoclinic
Space group	$P2_1/c$ (14)	$P2_1/c$ (14)
$a$ [ $\text{\AA}$ ]	9.030(1)	9.0136(18)
$b$ [ $\text{\AA}$ ]	12.977(1)	12.960(6)
$c$ [ $\text{\AA}$ ]	6.405(1)	6.3936(13)
$\alpha$ [ $^\circ$ ]	90	90
$\beta$ [ $^\circ$ ]	100.76(1)	100.77(3)
$\gamma$ [ $^\circ$ ]	90	90
$V$ [ $\text{\AA}^3$ ]		733.7(4)
$Z$		4
$\rho_{\text{calc}}$ [ $\text{g cm}^{-3}$ ]	1.803	1.812
$T$ [K]		294

Crystals are usually twinned<sup>[2]</sup>.

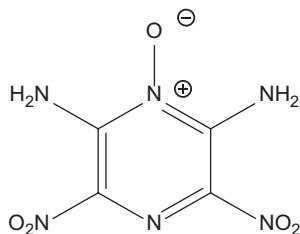
- [1] R. Gilardi, C. George, *The Structural Chemistry of Energetic Compounds*, ONR Annual Report, AD-A159203, 1st October 1983–1st October 1984.
- [2] R. Gilardi, R. J. Butcher, *Acta Cryst.*, **2001**, E57, 0738–0740.
- [3] D. S. Donald, *Tetraaminopyrazine, 2,3,5-Triamino-6-nitropyrazine, 2,6-Diamino-3,5-dinitropyrazine*, US Patent 3808209, 30th April 1974.
- [4] P. C. Hsu, G. Hust, M. McClelland, M. Gresshoff, *One-Dimensional Time to Explosion (Thermal Sensitivity) of ANPZ*, LLNL-TR-667280, Lawrence Livermore National Laboratory, California, USA, 25th April 1994.

## 2,6-Diamino-3,5-dinitropyrazine-1-oxide

Name [German, acronym]: 2,6-Diamino-3,5-dinitropyrazine-1-oxide, [3,5-dinitro-2,6-pyrazinediamin-1-oxid, ANPZ-O, LLM-105, NPEX-1, PZO]

Main (potential) use: Potential for use as an insensitive but thermally stable explosive

Structural formula:



	<b>LLM-105</b>
Formula	$\text{C}_4\text{H}_4\text{N}_6\text{O}_5$
Molecular mass [g mol <sup>-1</sup> ]	216.11
Appearance at RT	Brilliant yellow powder <sup>[23]</sup>
IS [cm]	<p>117<sup>[1]</sup>, &gt;320 cm (US drop hammer)<sup>[8]</sup>, Rotter F of I = 47–76<sup>[8]</sup>,  <math>H_{50} = 117 \text{ cm}</math><sup>[12]</sup>, DH<sub>50</sub> = 104 cm<sup>[15]</sup>, F of I = 54 (RDX = 80)<sup>[17]</sup>, 20 (BAM,      1 of 6)<sup>[18]</sup>, 91 cm<sup>[20]</sup>, <math>H_{50} = 117 \text{ cm}</math> (2 kg mass)<sup>[21]</sup>, &gt;26<sup>[22]</sup>, <math>A_{d1} = 32\%</math>,  <math>A_{d2} = 76\%</math>, LL = 1.3 m, <math>A_{50\ d1} = 3.8 \text{ m}</math>, <math>A_{50\ d2} = 1.9</math><sup>[26]</sup>, 50 cm<sup>[27]</sup></p> <p>99.6% purity, 1.9197 g cm<sup>-3</sup> crystal density, <math>H_{50} &gt; 112.2 \text{ cm}</math>, impact sensitivity 0%<sup>[6]</sup></p> <p>99.62% purity, 5 kg hammer, 1.9152 g cm<sup>-3</sup> crystal density, <math>H_{50} = 103.9 \text{ cm}</math>, impact sensitivity 4%<sup>[6]</sup></p> <p>99.41% purity, 5 kg hammer, 1.9134 g cm<sup>-3</sup> crystal density, <math>H_{50} = 48.2 \text{ cm}</math><sup>[6]</sup></p> <p>99.41% purity, 5 kg hammer, 1.9117 g cm<sup>-3</sup> crystal density, <math>H_{50} = 44.8 \text{ cm}</math><sup>[6]</sup></p> <p>99.55% purity, 5 kg hammer, 1.9065 g cm<sup>-3</sup> crystal density, <math>H_{50} &gt; 112.2 \text{ cm}</math><sup>[6]</sup></p> <p>(See reference [6] for further details of the effects of crystal surface defects, crystal sizes and crystal integrity on IS)</p>

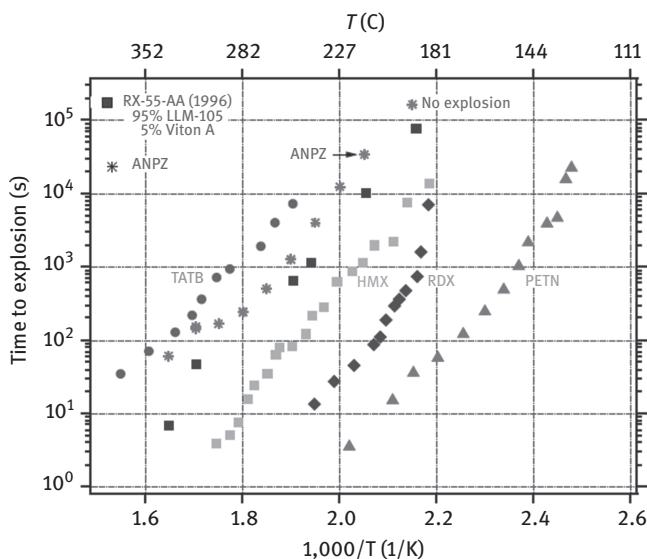
	LLM-105 particles prepared by different routes and with different morphologies <sup>[16]</sup> :																		
	<table border="1"> <thead> <tr> <th>Preparation method</th><th>Morphology (average size, <math>\mu\text{m}</math>)</th><th>Drop hammer, DH50 (cm)</th></tr> </thead> <tbody> <tr> <td>Original (nonrecrystallized)</td><td>80</td><td>115–120</td></tr> <tr> <td>Slow recryst. from DMSO/<math>\text{H}_2\text{O}</math></td><td>Sharp needles, 60</td><td>105</td></tr> <tr> <td>Crash precipitate from DMSO/cold <math>\text{H}_2\text{O}</math></td><td>Small particles, 2</td><td>60</td></tr> <tr> <td>Crash precipitate from butyrolactone/xylene soln.</td><td>Rounded granules and small fines, 40 + 2</td><td>55</td></tr> <tr> <td>Material from slow recryst. from DMSO/<math>\text{H}_2\text{O}</math> then subjected to 22 h milling</td><td>Fractured granules, 2</td><td>80</td></tr> </tbody> </table>	Preparation method	Morphology (average size, $\mu\text{m}$ )	Drop hammer, DH50 (cm)	Original (nonrecrystallized)	80	115–120	Slow recryst. from DMSO/ $\text{H}_2\text{O}$	Sharp needles, 60	105	Crash precipitate from DMSO/cold $\text{H}_2\text{O}$	Small particles, 2	60	Crash precipitate from butyrolactone/xylene soln.	Rounded granules and small fines, 40 + 2	55	Material from slow recryst. from DMSO/ $\text{H}_2\text{O}$ then subjected to 22 h milling	Fractured granules, 2	80
Preparation method	Morphology (average size, $\mu\text{m}$ )	Drop hammer, DH50 (cm)																	
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Material from slow recryst. from DMSO/ $\text{H}_2\text{O}$ then subjected to 22 h milling	Fractured granules, 2	80																	
	$H_{50} = 85 \text{ cm}$ (needle shape, 50 mg sample, 35 tests, 2.5 kg mass, CGY instrument) <sup>[23]</sup> , $H_{50} = 115 \text{ cm}$ (cubic morphology, 50 mg sample, 35 tests, 2.5 kg mass, CGY instrument) <sup>[23]</sup>																		
FS [N]	Insensitive <sup>[2]</sup> , $p_{\text{fr,LL}} = 400 \text{ MPa}$ <sup>[7,26]</sup> , $p_{\text{fr,50\%}} = 480 \text{ MPa}$ <sup>[7,26]</sup> , Rotter test (FoF) = 54 <sup>[8]</sup> , 36 <sup>[15]</sup> , F of F = 5.2 (insensitive) <sup>[17]</sup> , 360 (BAM, $1/\rho$ ) <sup>[18]</sup> , $0/_{10}$ @ 36.0 kg <sup>[20]</sup> , >360 <sup>[22,27]</sup>																		
ESD [J]	Insensitive <sup>[2]</sup> , 4.5 (not 0.45) <sup>[17]</sup> , 0.60 (OZM apparatus) <sup>[18]</sup> , $0/_{10}$ @ 1.0 J, 510 $\Omega$ <sup>[20]</sup> , 0.0366 <sup>[27]</sup>																		
N [%]	38.89																		
$\Omega(\text{CO}_2)$ [%]	-37.02																		
$T_{\text{m.p.}}$ [ $^\circ\text{C}$ ]	342 <sup>[2]</sup> , 333.5 <sup>[9]</sup> , 210 (dec.) <sup>[22]</sup>																		
$T_{\text{dec.}}$ [ $^\circ\text{C}$ ]	260 <sup>[3]</sup> , 354 <sup>[19,28]</sup> , 361 (DSC) <sup>[20]</sup> , 297.77 (exo, onset), 330.33 (exo, peak 1 max), 342.80 (exo, peak 2 max) (DSC @ 2 K/min, Al pan, pierced lid) <sup>[14]</sup> , 342 <sup>[18]</sup> , 216.1 <sup>[21]</sup> , 310 <sup>[22]</sup> , 300.5–360.4 (exothermic dec., $T_{\text{max}} = 345.3$ , DSC @ 5 $^\circ\text{C}/\text{min}$ ) <sup>[23]</sup> , 361 (peak max, DSC @ 10 $^\circ\text{C}/\text{min}$ , hermetic pan, pinhole lid) <sup>[25]</sup> , 354 (peak max, DSC @ 10 $^\circ\text{C}/\text{min}$ , standard pan) <sup>[25]</sup>																		
$\rho$ [ $\text{g cm}^{-3}$ ]	1.911 (@ 296 K) <sup>[4]</sup> , 1.91 <sup>[9,18,21]</sup> , 1.919 <sup>[12]</sup> , 1.9097 (99.8 TMD) <sup>[15]</sup> , 1.913 <sup>[23]</sup> , 1.918 (crystal) <sup>[19]</sup> , 1.918 <sup>[20]</sup> , 1.913 (X-ray) <sup>[22]</sup> , 1.92 <sup>[28]</sup>																		
Heat of formation	-12.97 kJ/mol ( $\Delta_f H^\circ$ ) <sup>[2]</sup> , -60.02 kJ $\text{kg}^{-1}$ ( $\Delta_f H^\circ$ ) <sup>[2]</sup> , 129.07 kJ/mol (calcd., isodesmic) <sup>[4]</sup> , -3.10 kcal/mol ( $\Delta_f H(s)$ ) <sup>[12]</sup> , 13.0 kJ/mol ( $\Delta_f H$ ) <sup>[13]</sup> , -13 kJ/mol <sup>[27]</sup>																		

	Calcd. (EXPLO5 6.04) [EXPLO5 6.03]	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^\circ [\text{kJ kg}^{-1}]$	4,489 [4,502] <sup>[18]</sup>	4,900 (calcd., K-J) <sup>[5]</sup> 1.17 kcal/g ( $Q_{\max}$ , calcd.) <sup>[12]</sup>	
$T_{\text{ex}} [\text{K}]$	3,200 [3,199] <sup>[18]</sup>	3,587 (@ 1.913 g cm <sup>-3</sup> , calcd. CHEETAH 2.0) <sup>[22]</sup>  2,828 (@ 1.913 g cm <sup>-3</sup> , $\Delta H_f = -13 \text{ kJ/mol}$ , calcd., JAGUAR) <sup>[24]</sup>	
$p_{\text{C-J}} [\text{kbar}]$	312 [317] <sup>[18]</sup>	314.4 (calcd., K-J) <sup>[4]</sup>  316 (@ 1.919 g cm <sup>-3</sup> , calcd.) <sup>[12]</sup>  35 GPa <sup>[21]</sup>  33.4 GPa (calcd., CHEETAH 2.0) <sup>[22]</sup>  33.38 (@ 1.913 g cm <sup>-3</sup> , calcd. CHEETAH 2.0) <sup>[22]</sup>  30.4 GPa (@ 1.913 g cm <sup>-3</sup> , $\Delta H_f = -13 \text{ kJ/mol}$ , calcd., JAGUAR) <sup>[24]</sup>  32.72 GPa (calcd., CHEETAH 7.0) <sup>[27]</sup>	359 <sup>[2]</sup>
VoD [m s <sup>-1</sup> ]	8,533 (@ 1.913 g cm <sup>-3</sup> , $\Delta_f H = 13 \text{ kJ mol}^{-1}$ )  8,641 (@ 1.91 g cm <sup>-3</sup> ) <sup>[18]</sup>	8,529 (@ 1.911 g cm <sup>-3</sup> , calcd., K-J) <sup>[4]</sup>  8,280 (@ 1.919 g cm <sup>-3</sup> , calcd.) <sup>[12]</sup>	8,560 (@ 1.913 g cm <sup>-3</sup> ) <sup>[4]</sup>  8,120 (@ 1.80 g cm <sup>-3</sup> , 95% ANZPO, 5% Viton A) <sup>[23]</sup>

		8,557 (@ 1.913 g cm <sup>-3</sup> , calcd. CHEETAH 2.0) <sup>[22]</sup>  8,560 (@ 1.913 g cm <sup>-3</sup> , $\Delta H_f = -13 \text{ kJ/mol}$ , calcd., JAGUAR) <sup>[24]</sup>  8,667 (@ 1.881 g cm <sup>-3</sup> , calcd., CHEETAH 7.0) <sup>[27]</sup>	
$V_0$ [L kg <sup>-1</sup> ]	701 [706] <sup>[18]</sup>	60.43 mol × 10 <sup>3</sup> (g) per cm <sup>3</sup> LLM-105 @ 0.1 MPa (@ 1.913 g cm <sup>-3</sup> , calcd. CHEETAH 2.0) <sup>[22]</sup>	

5 s explosion $T$ [°C] Ignition $T$ [°C]	328 <sup>[17]</sup>
Vacuum stability test [cm <sup>3</sup> /h]	STANAG 4147 test 1B, total gas evolved after 40 h @ 100 °C, values in cc): 0.4348 <sup>[27]</sup>
Vapor pressure [atm @ °C]	$8.50 \times 10^{-16}$ Torr @ 25 °C (est.) <sup>[25,27]</sup> , $9.15 \times 10^{-13}$ Torr @ 70 °C (est.) <sup>[25,27]</sup> , $50.4 \times 10^{-10}$ Torr @ 100 °C (est.) <sup>[25,27]</sup>
Burn rate [mm/s]	
Solubility [g/mL]	$1.4 \times 10^{-2}$ mg/mL in H <sub>2</sub> O @ 25 °C <sup>[25]</sup>
Compatibility	VTS compatibility (STANAG 4147 test 1B, 2.5 g of compound 1 mixed with 2.5 g of compound 2, total gas evolved after 40 h @ 100 °C, values in cc) <sup>[1]</sup> : 0.7201 (TNBA), 0.5184 (DNMT), 1.7547 (PiPE), 1.6351 (DNP), 0.6147 (DNGU), – (HK-56), 0.3372 (HMX) concluding that all are compatible with LLM-105 <sup>[27]</sup>
$\Delta H_{\text{dec.}}$ [kJ/mol]	266.5 <sup>[14]</sup> , 598.2 J/g (energy output during dec.) <sup>[23]</sup> , 1433 J/g (DSC @ 10 °C/min, hermetic pan, pinhole lid) <sup>[25]</sup> , 678 J/g (DSC @ 10 °C/min, standard pan) <sup>[25]</sup>
$\Delta H_{\text{vap}}$ [kJ/mol]	163.8 (est.) <sup>[25,27]</sup>
CRT @ 120 °C	0.2 cc/g <sup>[20]</sup>
$K_{\text{ow}}$	0.058 (est.) <sup>[25]</sup> , $\log K_{\text{ow}} = -1.2$ (est.) <sup>[25]</sup>
$K_{\text{oc}}$	124 (measured) <sup>[25]</sup> , 209 (predicted) <sup>[25]</sup> , $\log K_{\text{oc}} = 2.09$ (est.) <sup>[25]</sup>
ODTX	see figure 6 below <sup>[20]</sup>

Data from ref.<sup>[20]</sup>:



**Fig. 6:** ODTX results of ANPZ and TATB, HMX, RDX and PETN<sup>[20]</sup>.

	LLM-105 <sup>[10]</sup>	LLM-105 <sup>[4]</sup>	LLM-105 <sup>[11]</sup>
Chemical formula	C <sub>4</sub> H <sub>4</sub> N <sub>6</sub> O <sub>5</sub>	C <sub>4</sub> H <sub>4</sub> N <sub>6</sub> O <sub>5</sub>	C <sub>4</sub> H <sub>4</sub> N <sub>6</sub> O <sub>5</sub>
Molecular weight [g mol <sup>-1</sup> ]	216.13	216.13	216.13
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	P2 <sub>1</sub> /n (no. 14)	P2 <sub>1</sub> /n (no. 14)	P2 <sub>1</sub> /n (no. 14)
<i>a</i> [Å]	5.709(2)	5.722(2)	5.7430(11)
<i>b</i> [Å]	15.844(8)	16.875(6)	15.825(3)
<i>c</i> [Å]	8.416(3)	8.428(3)	8.3930(17)
$\alpha$ [°]	90	90	90
$\beta$ [°]	101.14(3)	101.05(1)	100.97(3)
$\gamma$ [°]	90	90	90
<i>V</i> [Å <sup>3</sup> ]	747.0(6)	751.379	748.8(3)
<i>Z</i>	4	4	4
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.922	1.911	1.917
<i>T</i> [K]	293	296	293

Crystals prepared by the method described in reference<sup>[23]</sup> show a cubic morphology with smooth particle surfaces with an average particle size of 40 µm<sup>[23]</sup>; particle size increased as the reaction temperature was increased<sup>[23]</sup>; crystal morphology changes from cubic to cubic rod shape on increasing the stirring rate<sup>[23]</sup>; cubic rod shape morphology was obtained according to reference<sup>[23]</sup> @ 500 rpm/min<sup>[23]</sup>.

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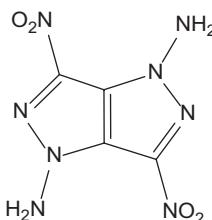
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**1,4-Diamino-3,6-dinitropyrazolo[4,3-c]pyrazole**

Name [German, acronym]: 3,6-Dinitropyrazolo[4,3-c]pyrazole-1,4-diamine  
[LLM-119]

Main (potential) use: secondary explosive

Structural formula:



	LLM-119	
Formula	C <sub>4</sub> H <sub>4</sub> N <sub>8</sub> O <sub>4</sub>	
Molecular mass [g mol <sup>-1</sup> ]	228.13	
Appearance at RT	Brown crystals <sup>[2]</sup>	
IS [J]	DH <sub>50</sub> = 24 cm <sup>[3]</sup> , 15 <sup>[2]</sup> , 7 <sup>[5]</sup>	
FS [N]	Not friction sensitive as tested <sup>[3]</sup> , 280 <sup>[2]</sup> , 120 <sup>[5]</sup>	
ESD [J]	Not spark sensitive as tested <sup>[3]</sup>	
N [%]	49.12	
Ω(CO <sub>2</sub> ) [%]	-42.1	
T <sub>m.p.</sub> [°C]		
T <sub>dec.</sub> [°C]	253 (exo, DSC) <sup>[1,3]</sup> , 526 K (exo peak, DSC) <sup>[4]</sup> , 240 <sup>[2]</sup> , 230 (onset) <sup>[5]</sup>	
ρ [g cm <sup>-3</sup> ]	1.835 <sup>[1]</sup> , 1.845 (X-ray) <sup>[3,3]</sup> , 1.9 (calcd., MOLPAK) <sup>[4]</sup> , 2.0 (calcd., group additivity method) <sup>[4]</sup> , 1.84 (X-ray @ 296 K) <sup>[2]</sup> , 1.84 (gas pycnometer) <sup>[5]</sup>	
Heat of formation	114 kcal/mol (ΔH, calcd.) <sup>[1,3]</sup> , 510 kJ/mol (calcd., HF corrected) <sup>[4]</sup> , 584 kJ/mol (calcd., DFT) <sup>[4]</sup> , 460 kJ/mol (ΔH <sub>f</sub> , calcd.) <sup>[2]</sup> , 467 kJ/mol (ΔH <sub>f</sub> , heat of form.) <sup>[5]</sup>	
Calcd. (EXPL05 6.01)	Lit. values	Exptl.
-Δ <sub>ex</sub> U <sup>o</sup> [kJ kg <sup>-1</sup> ]		
T <sub>ex</sub> [K]		

$p_{C_J}$ [kbar]	33.9 GPa (@ 1.84 g cm <sup>-3</sup> ) <sup>[5]</sup>	32.3 GPa (@ 1.84 g cm <sup>-3</sup> , calcd., K-J) <sup>[2]</sup>	
VoD [m s <sup>-1</sup> ]	8,864 (@ 1.84 g cm <sup>-3</sup> ) <sup>[5]</sup>	8,404 (@ 1.84 g cm <sup>-3</sup> , calcd., K-J) <sup>[2]</sup>	
$V_0$ [L kg <sup>-1</sup> ]			
$I_{sp}$ [s]	256 <sup>[5]</sup>		
Metal acceleration energy	1.1× that of HMX (predicted) <sup>[4]</sup>		

	LLM-119 <sup>[2]</sup>
Chemical formula	C <sub>4</sub> H <sub>4</sub> N <sub>8</sub> O <sub>4</sub>
Molecular weight [g mol <sup>-1</sup> ]	228.15
Crystal system	Orthorhombic
Space group	Pbca
$a$ [\text{\AA}]	9.082(2)
$b$ [\text{\AA}]	5.4849(13)
$c$ [\text{\AA}]	16.575(4)
$\alpha$ [ $^\circ$ ]	90
$\beta$ [ $^\circ$ ]	90
$\gamma$ [ $^\circ$ ]	90
$V$ [\text{\AA}³]	825.7(3)
$Z$	4
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.835
$T$ [K]	296

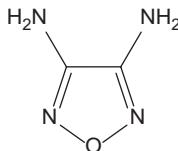
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## 3,4-Diaminofurazan

Name [German, acronym]: Diaminofurazan, 3,4-diamino-1,2,5-oxadiazole,  
1,2,5-oxadiazole-3,4-diamine [3,4-diaminofurazan, DAF]

Main (potential) use: Of interest in cocrystals since DAF has been shown to modify the properties of energetic materials<sup>[2]</sup>

### Structural formula:



	DAF		
Formula	$\text{C}_2\text{H}_4\text{N}_4\text{O}$		
Molecular mass [g mol <sup>-1</sup> ]	100.08		
Appearance at RT	White-beige powder or crystals		
IS [J]	$\text{DH}_{50} \geq 145 \text{ cm}$ (2 mg sample in nonhermetic DSC pans, 5 lb mass, nonstandard apparatus, cf. 29 cm for $\epsilon$ -CL-20 and 55 cm for $\beta$ -HMX using this apparatus) <sup>[2]</sup>		
N [%]	55.98		
$\Omega(\text{CO}_2)$ [%]	-79.9		
$T_{\text{m.p.}}$ [°C]	180 <sup>[2]</sup> , 177.4 (onset, DSC @ 10 °C/min, hermetic Al pans, N <sub>2</sub> purge) <sup>[2]</sup> , 178–183 <sup>[3]</sup>		
$T_{\text{b.p.}}$ [°C]	$304.0 \pm 45.0$ @ 760 mm Hg <sup>[3]</sup>		
$T_{\text{phase transition}}$ [°C]			
$T_{\text{dec.}}$ [°C]	250 <sup>[2]</sup> , 244.5 (onset, DSC @ 10 °C/min, hermetic Al pans, N <sub>2</sub> purge) <sup>[2]</sup>		
$\rho$ [g cm <sup>-3</sup> ]	1.61 <sup>[2]</sup> , 1.6 ± 0.1 <sup>[3]</sup>		
Heat of formation			
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^\circ$ [kJ kg <sup>-1</sup> ]			
$T_{\text{ex}}$ [K]			

$p_{\text{C-J}}$ [kbar]		20.835 GPa (@ crystal $\rho$ @ RT, calcd., CHEETAH 7.0) <sup>[2]</sup>	
VoD [ $\text{m s}^{-1}$ ]		7,502 (@ crystal $\rho$ @ RT, calcd., CHEETAH 7.0) <sup>[2]</sup>	
$V_0$ [ $\text{L kg}^{-1}$ ]			
Vapor pressure [Pa]	$0.0 \pm 0.6$ mm Hg (@ 25 °C) <sup>[3]</sup>		
Flash point [°C]	$137.7 \pm 28.7$ <sup>[3]</sup>		
Refraction index	1.655 <sup>[3]</sup>		

	<b>DAF<sup>[1]</sup></b>
Chemical formula	C <sub>2</sub> H <sub>4</sub> N <sub>4</sub> O
Molecular weight [g mol <sup>-1</sup> ]	100.04
Crystal system	Monoclinic
Space group	C2/c
$a$ [\AA]	3.6035(3)
$b$ [\AA]	11.141(2)
$c$ [\AA]	10.329(1)
$\alpha$ [°]	90
$\beta$ [°]	94.80(11)
$\gamma$ [°]	90
$V$ [\AA <sup>3</sup> ]	413.2(1)
$Z$	4
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.61
$T$ [K]	20 °C

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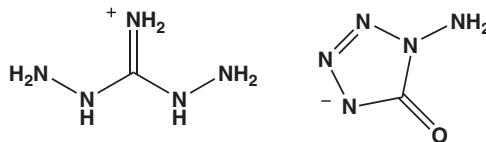
[3] 3,4-Diaminofurazan [https://www.chemsrc.com/en/cas/17220-38-1\\_78109.html](https://www.chemsrc.com/en/cas/17220-38-1_78109.html)

## Diaminoguanidinium 1-aminotetrazol-5-oneate

Name [German, acronym]: Diaminoguanidinium 1-aminotetrazol-5-oneate  
[ATO · DAG]

Main (potential) use: Secondary (high) explosive

Structural formula:



	<b>ATO · DAG</b>
Formula	C <sub>2</sub> H <sub>10</sub> N <sub>10</sub> O
Molecular mass [g mol <sup>-1</sup> ]	190.20
Appearance at RT	Yellow powder <sup>[1]</sup>
IS [J]	>40 <sup>[1]</sup>
N [%]	73.7
Ω(CO <sub>2</sub> ) [%]	-67.3
T <sub>m.p.</sub> [°C]	153.0 (DSC-TG @ 10 °C/min) <sup>[1]</sup>
T <sub>dec.</sub> [°C]	220.7 (DSC-TG @ 10 °C/min) <sup>[1]</sup>
ρ [g cm <sup>-3</sup> ]	1.534 (@ 298 K) <sup>[1]</sup>
Heat of formation	608.36 kJ/mol (Δ <sub>f</sub> H°, calcd.) <sup>[1]</sup> , 3,198.5 kJ kg <sup>-1</sup> (Δ <sub>f</sub> H°, calcd.) <sup>[1]</sup>
	Calcd. (K-J)
	Exptl.
-Δ <sub>ex</sub> U° [kJ kg <sup>-1</sup> ]	
T <sub>ex</sub> [K]	
p <sub>C-J</sub> [kbar]	284 <sup>[1]</sup>
VoD [m s <sup>-1</sup> ]	8,410 (@ TMD) <sup>[1]</sup>
V <sub>0</sub> [L kg <sup>-1</sup> ]	

	<b>ATO-DAG<sup>[1]</sup></b>
Chemical formula	C <sub>2</sub> H <sub>10</sub> N <sub>10</sub> O
Molecular weight [g mol <sup>-1</sup> ]	190.20
Crystal system	Monoclinic

Space group	$P2_1/n$
$a$ [Å]	7.0441(5)
$b$ [Å]	12.0324(11)
$c$ [Å]	10.1093(8)
$\alpha$ [°]	90
$\beta$ [°]	105.964(2)
$\gamma$ [°]	90
$V$ [Å <sup>3</sup> ]	823.79(12)
$Z$	4
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.534
$T$ [K]	298

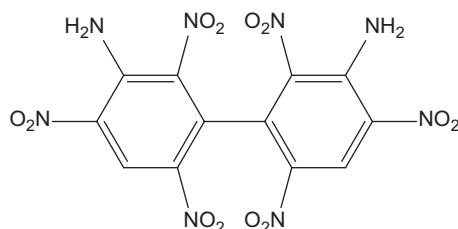
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### 3,3'-Diamino-2,2',4,4',6,6'-hexanitrobiphenyl

Name [German, acronym]: Dipicramide, dipicrylamide, diaminohexanitrobiphenyl [dipikramid, DIPAM]

Main (potential) use: Flexible linear-shaped charges<sup>[6]</sup>, metal-sheathed mild detonating fuze for stage separation in Polaris missile (MDF)<sup>[6]</sup>, used when explosive must withstand high temperatures<sup>[6]</sup>, potential for use in high temperature mild detonating fuses<sup>[11]</sup>

Structural formula:



	DIPAM												
Formula	C <sub>12</sub> H <sub>6</sub> N <sub>8</sub> O <sub>12</sub>												
Molecular mass [g mol <sup>-1</sup> ]	454.22												
Appearance at RT	Yellow solid <sup>[6]</sup> , bright yellow crystalline solid <sup>[10]</sup> , orange-brown powder (crude product) <sup>[11]</sup> , microcrystalline powder (purified) <sup>[11]</sup>												
IS [J]	<p>185 cm (NOL)<sup>[1]</sup>, 85 cm (LANL)<sup>[1]</sup>, <math>H_{50} = 67</math> cm (2.5 kg mass, type 12 tool)<sup>[4]</sup>, 95 cm (50% point, type 12 tool, 2.5 kg mass, sandpaper)<sup>[9]</sup>, 114 cm (50% point, type 12 tool, 2.5 kg mass, particle size &gt;105 µm, sandpaper)<sup>[9]</sup>, 132 cm (<math>\sigma = 0.23</math>, type 12 tool, ERL machine; cf. <math>H_{50}</math> of TNT = 160 cm, tetryl = 32 cm, RDX = 24 cm)<sup>[11]</sup>, <math>H_{50} = 95</math> cm (5 kg mass, LLNL)<sup>[13]</sup>, <math>H_{50} = 85</math> cm (2.5 kg mass, LANL)<sup>[13]</sup>, <math>H_{50} = 85.1 \pm 0.06</math> cm (type 12)<sup>[16]</sup>, <math>H_{50} = 95.5 \pm 0.04</math> cm (type 12B)<sup>[16]</sup>, <math>H_{50\%} = 67</math> cm (2.5 kg mass, type 12 tool, 35 mg sample in conical pile, 1 in<sup>2</sup> garnet paper)<sup>[18]</sup>, 95 cm (2.5 kg mass, P.A.)<sup>[19]</sup>, 95 cm (5 kg mass/TL 12, ERL)<sup>[19]</sup></p> <p>Rotter impact data: 27 mg sample, Bruceton method/25 drop run to obtain <math>H_{50\%}</math>; initiation criteria = 1 mL gas evolved or 0.5 mL accompanied by smoke or evidence of burning in the sample; data from ref.<sup>[15]</sup>:</p> <table border="1"> <thead> <tr> <th colspan="2">Rotter impact data</th> <th colspan="2">US data</th> </tr> <tr> <th>F of I</th> <th>Gas evolved (mL)</th> <th>NSWC/NOL, ERL type 12</th> <th>NWC B.M. type 12</th> </tr> </thead> <tbody> <tr> <td>80</td> <td>6.0</td> <td>121</td> <td>67</td> </tr> </tbody> </table>	Rotter impact data		US data		F of I	Gas evolved (mL)	NSWC/NOL, ERL type 12	NWC B.M. type 12	80	6.0	121	67
Rotter impact data		US data											
F of I	Gas evolved (mL)	NSWC/NOL, ERL type 12	NWC B.M. type 12										
80	6.0	121	67										

ESD [J]	Extremely insensitive to electrostatic discharge <sup>[7]</sup> , >32 kJ <sup>[7]</sup>		
N [%]	24.67		
$\Omega(\text{CO}_2)$ [%]	-52.8		
$T_{\text{m.p.}}$ [°C]	306 (dec., Thomas Hoover capillary melting point apparatus @ 2 °C/min) <sup>[2]</sup> , 304 <sup>[2,7,13]</sup> , 306 <sup>[6]</sup> , 305 (dec., recryst. from THF/toluene) <sup>[10]</sup> , 298–299 (dec., recryst.) <sup>[11]</sup> , 299 (dec., microcryst. yellow powder) <sup>[11]</sup> , 298 (recryst.) <sup>[11]</sup> , 303 <sup>[16]</sup>		
$T_{\text{dec.}}$ [°C]	305 (recryst. from THF/toluene) <sup>[10]</sup> , 298–299 (recryst.) <sup>[11]</sup> , 316 <sup>[13]</sup>		
$\rho$ [g cm <sup>-3</sup> ]	Bulk $\rho$ of crystalline DIPAM in range 0.26–0.77 is possible <sup>[10]</sup> , bulk $\rho$ = 0.26–0.35 (crude DIPAM dissolved in acetone, boiling and addition of EtOH, more rapid concentration and addition of EtOH the smaller the particle size and lower bulk $\rho$ ) <sup>[10]</sup> , 0.46 (bulk $\rho$ if recryst. form ethylene glycol) <sup>[10]</sup> , 0.38 (bulk $\rho$ , recryst. from THF/toluene) <sup>[10]</sup> , 0.5 (bulk $\rho$ , THF/toluene, 1:2, continuous extraction-recryst. apparatus) <sup>[10]</sup> , 0.48 (bulk $\rho$ , acetone/acetic acid, continuous extraction-recryst. apparatus) <sup>[10]</sup> , 0.55 (bulk $\rho$ , THF/CCl <sub>4</sub> , 2:1, continuous extraction-recryst. apparatus) <sup>[10]</sup> , 0.65 (bulk $\rho$ , THF/CCl <sub>4</sub> , 2:1, continuous extraction-recryst. apparatus, seeded with 0.55 g/mL material) <sup>[10]</sup> , 0.77 (bulk $\rho$ , THF/CCl <sub>4</sub> , 1:1, continuous extraction-recryst. apparatus, seeded with 0.65 g/mL material) <sup>[10]</sup> , 0.66 (THF/nitrobenzene, 1:1, Soxhlet) <sup>[10]</sup> , 1.79 (crystal) <sup>[11]</sup> , 1.79 <sup>[16,18]</sup> , 1.79 (TMD) <sup>[19]</sup>		
Heat of formation	-8.0 kcal/kg (enthalpy of form.) <sup>[3]</sup> , -27.6 kcal/mol ( $\Delta H_f$ , calcd., based on exptl. value of picramide) <sup>[11]</sup> , -28.84 kJ/mol ( $\Delta H_f$ ) <sup>[14]</sup> , -6.8 kcal/mol ( $\Delta H_f^\circ$ ) <sup>[16]</sup> , -6.80 kcal/mol ( $\Delta H_f^\circ$ ) <sup>[17]</sup> , -6.8 kcal/mol <sup>[19]</sup>		
Heat of combustion	$\Delta H^\circ_c = -1326.8 \text{ kcal/mol}$ <sup>[16]</sup> , -1,326.8 kcal/mol <sup>[19]</sup>		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^\circ$ [kJ kg <sup>-1</sup> ]		1,077 kcal/kg (@ 1.790 g cm <sup>-3</sup> , calcd.) [H <sub>2</sub> O vapor]) <sup>[3]</sup>  845 (calcd.) <sup>[11]</sup>  2,890 (@ 1.79 g cm <sup>-3</sup> , calcd., LOTUSES) <sup>[14]</sup>	1,077 kcal/kg (@ 1.790 g cm <sup>-3</sup> ) [H <sub>2</sub> O vapor]) <sup>[3]</sup>
$T_{\text{ex}}$ [K]		2,900 (@ 1.79 g cm <sup>-3</sup> , calcd., LOTUSES) <sup>[14]</sup>	

$p_{c,j}$ [kbar]		26.36 (@ 1.79 g cm <sup>-3</sup> , calcd., LOTUSES) <sup>[14]</sup>  250 (@ 1.80 g cm <sup>-3</sup> , calcd.) <sup>[18]</sup>  269 (@ 1.79 g cm <sup>-3</sup> ) <sup>[93]</sup>																																																						
VoD [m s <sup>-1</sup> ]		7,560 (@ 1.79 g cm <sup>-3</sup> , calcd., LOTUSES) <sup>[14]</sup>  7,570 (@ 1.80 g cm <sup>-3</sup> , calcd.) <sup>[18]</sup>  7,400 (@ 1.76 g cm <sup>-3</sup> ) <sup>[19]</sup>  7,738 (@ 1.79 g cm <sup>-3</sup> ) <sup>[19]</sup>																																																						
$V_0$ [L kg <sup>-1</sup> ]		988 (@ 1.79 g cm <sup>-3</sup> , calcd., LOTUSES) <sup>[14]</sup>																																																						
$I_{sp}$ [Ns g <sup>-1</sup> ]		2.16 (calcd., ISPBKW code) <sup>[17]</sup> , 2.17 (calcd., empirical) <sup>[17]</sup>																																																						
SSGT [cm]	<p>5.2 mm (NOL)<sup>[1]</sup></p> <p>TMD = 1.79, data from ref.<sup>[9]</sup></p> <table border="1"> <thead> <tr> <th rowspan="2">Loading pressure (kpsi)</th> <th colspan="2">Density (g/cm<sup>3</sup>)</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><math>s_m</math></th> <th>N</th> </tr> </thead> <tbody> <tr> <td>64</td> <td>1.750</td> <td>0.0128</td> <td>97.8</td> <td>7.081</td> <td>0.1255</td> <td>0.0625</td> <td>23</td> </tr> </tbody> </table> <p>TMD = 1.79, data from ref.<sup>[9]</sup></p> <table border="1"> <thead> <tr> <th rowspan="2">Loading pressure (kpsi)</th> <th colspan="2">Density (g/cm<sup>3</sup>)</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><math>s_m</math></th> <th>N</th> </tr> </thead> <tbody> <tr> <td>4</td> <td>1.216</td> <td>0.0077</td> <td>67.9</td> <td>5.233</td> <td>0.0485</td> <td>0.0281</td> <td>23</td> </tr> <tr> <td>16</td> <td>1.461</td> <td>0.0073</td> <td>81.6</td> <td>5.730</td> <td>0.0168</td> <td>0.0150</td> <td>23</td> </tr> </tbody> </table>				Loading pressure (kpsi)	Density (g/cm <sup>3</sup> )		% TMD	Sensitivity (DBG)				AVG.	S	AVG.	g	$s_m$	N	64	1.750	0.0128	97.8	7.081	0.1255	0.0625	23	Loading pressure (kpsi)	Density (g/cm <sup>3</sup> )		% TMD	Sensitivity (DBG)				AVG.	S	AVG.	g	$s_m$	N	4	1.216	0.0077	67.9	5.233	0.0485	0.0281	23	16	1.461	0.0073	81.6	5.730	0.0168	0.0150	23
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	AVG.	<i>s</i>		AVG.	<i>g</i>	<i>s<sub>m</sub></i>	<i>N</i>	
8	1.307	0.0553	73.0	5.619	0.0788	0.0394	23	
16	1.478	0.0228	82.6	5.988	0.0208	0.0132	23	
32	1.627	0.0230	90.9	6.424	0.0365	0.0234	23	
64	1.784	0.0037	99.7	7.539	0.0808	0.0419	23	
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	AVG.	<i>s</i>		AVG.	<i>g</i>	<i>s<sub>m</sub></i>	<i>N</i>	
8	1.356	0.0257	75.8	5.281	0.0435	(illegible)	20	
32	1.674	0.0053	93.5	6.236	0.0338	0.0228	20	
8	1.394	0.0362	77.9	5.256	0.0757	0.0446	20	
32	1.662	0.0865	92.8	6.358	0.0156	0.0216	20	
TMD = 1.79, DIPAM particle size >105 µm, tested at -315 °F <sup>[9]</sup> :								
Loading pressure (kpsi)	Density (g/cm <sup>3</sup> )		% TMD	Sensitivity (DBG)				<i>N</i>
	AVG.	<i>s</i>		AVG.	<i>g</i>	<i>s<sub>m</sub></i>	<i>N</i>	
8	1.290	0.0164	72.1	6.704	0.2693	0.1584	18	
32	1.608	0.0125	89.8	7.297	0.1170	0.0672	18	
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	AVG.	<i>s</i>		AVG.	<i>g</i>	<i>s<sub>m</sub></i>	<i>N</i>	
32	1.627	0.0062	90.9	6.312	0.0290	0.0216	20	
35	1.642	0.0057	91.7	6.372	0.0050	0.0040	20	

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5 s explosion T [°C] Autoignition T [°C]	504 (1 s) <sup>[19]</sup> , 305 (10 s) <sup>[1]</sup>																																																						
Vacuum stability test [cm <sup>3</sup> /h]	<p>@ 200 °C, total gas evolved (cm<sup>3</sup>/g) @ STP/time of exposure (days)<sup>[5]</sup>:      2.5/2, 3.3/7, 4.2/14, 5.0/21, 5.9/28, 6.9/35, 7.9/42, 9.4/49,      10.4/56, 11.7/63, 12.8/70, 14.2/77, 15.6/84<sup>[5]</sup></p> <p>0.65 cc (20 min surge), 1.26 cc/g/h (2 h period) @ 260 °C<sup>[10]</sup>,      0.3 cc/g/h @ 230 °C (6 h period)<sup>[11]</sup>, 0.3 cc/g/h @ 245 °C      (2 h period)<sup>[11]</sup>, 3.5 cc/g/h @ 260 °C (2 h period)<sup>[11]</sup></p> <p>@ 150 °C, total gas evolved (cm<sup>3</sup>/g) @ STP/time of exposure (days)<sup>[12]</sup>:      0.2/2, 0.4/7, 0.5/14, 0.5/21, 0.6/28, 0.7/35, 0.7/42, 0.8/49, 0.8/56,      0.9/63, 0.9/70, 1.0/77, 1.0/84, 1.0/91<sup>[12]</sup></p> <p>0.1 mL/g/40 h @ 120 °C<sup>[19]</sup></p>																																																						
Thermal stability	0.2–0.3% dec./h @ 260 °C <sup>[6]</sup> , 0.1%/g/48 h @ 120 °C <sup>[13]</sup>																																																						
Volatility	1.0 mm pressure, 0% mass loss (evacuated Abderhalden's drying apparatus over boiling nitrobenzene (~210 °C), mass loss determined for 30 min interval) <sup>[11]</sup>																																																						
Solubility [g/mL]	Soluble in acetone <sup>[6,10]</sup> , solubility increases: acetone < THF < dioxane < nitrobenzene < DMF <sup>[10]</sup> , recryst. possible from THF/toluene, THF/CCl <sub>4</sub> , THF/xylene, THF/nitrobenzene, acetone/acetic acid, acetone/CCl <sub>4</sub> , dioxane/toluene and dioxane/xylene <sup>[10]</sup> , 10 g/100 mL in boiling THF <sup>[10]</sup>																																																						
Reflectance tests	<p>Reflectance tests @ 10,600 Å (continuous-wave yttrium garnet aluminum laser, pressed explosive)<sup>[8]</sup>:</p> <table border="1"> <thead> <tr> <th>Material</th> <th>Particle size, mesh</th> <th>Loading pressure (10<sup>3</sup> psi)</th> <th>Reflectance (%)</th> </tr> </thead> <tbody> <tr> <td>DIPAM</td> <td>Unknown</td> <td>10</td> <td>94.0</td> </tr> </tbody> </table>	Material	Particle size, mesh	Loading pressure (10 <sup>3</sup> psi)	Reflectance (%)	DIPAM	Unknown	10	94.0																																														
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Heat capacity [cal/g °C]	$C_p = 0.235 + (6.2 \times 10^{-4})T - (4.75 \times 10^{-7})T^2$ (@ density = 1.79 g cm <sup>-3</sup> ) <sup>[16]</sup>																																																						

Laser ignition	754 J/cm <sup>2</sup> /0.250 µs (threshold) <sup>[19]</sup>
Brisance	Dent test: 0.119 in <sup>[19]</sup> , fragment: 2,250 m/s (@ 1.79 g cm <sup>-3</sup> ) <sup>[19]</sup>
	<b>DIPAM<sup>[10]</sup></b>
Chemical formula	C <sub>12</sub> H <sub>6</sub> N <sub>8</sub> O <sub>12</sub>
Molecular weight [g mol <sup>-1</sup> ]	454
Crystal system	Monoclinic
Space group	
a [Å]	
b [Å]	
c [Å]	
α [°]	90
β [°]	95
γ [°]	90
V [Å <sup>3</sup> ]	
Z	
ρ <sub>calc</sub> [g cm <sup>-3</sup> ]	
T [K]	

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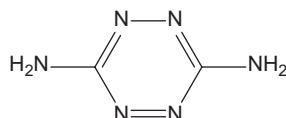
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## 3,6-Diamino-1,2,4,5-tetrazine

Name [German, acronym]: Diaminotetrazine, *sym*-diaminotetrazine [3,6-diamino-1,2,4,5-tetrazin, DATz]

Main (potential) use: gas generant

Structural formula:



	3,6-Diamino-1,2,4,5-tetrazine		
Formula	C <sub>2</sub> H <sub>4</sub> N <sub>6</sub>		
Molecular mass [g mol <sup>-1</sup> ]	112.10		
Appearance at RT	Brown crystals <sup>[2]</sup> , red solid (crude product) <sup>[4]</sup> , orange-red microcrystalline on recryst. from dioxane and from water <sup>[4]</sup>		
<i>N</i> [%]	74.97		
$\Omega(\text{CO}_2)$ [%]	-85.6		
<i>T</i> <sub>m.p.</sub> [°C]	Does not melt up to 300 °C but does sublime in region of 200–240 °C depending on the rate of heating <sup>[4]</sup>		
<i>T</i> <sub>dec.</sub> [°C]	342.17 (exo, DSC @ 10 °C/min) <sup>[3]</sup> , 351.15 (exo, DTG) <sup>[3]</sup> , 265.15 (mass loss begins, 366.48 °C mass loss ends, TG) <sup>[3]</sup>		
$\rho$ [g cm <sup>-3</sup> ]	1.611 (X-ray @ 295 K) <sup>[2]</sup> , 1.605 (X-ray) <sup>[3]</sup>		
Heat of formation			
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{\text{ex}} U^\circ$ [kJ kg <sup>-1</sup> ]			
<i>T</i> <sub>ex</sub> [K]			
$p_{\text{C}_7}$ [kbar]			
VoD [m s <sup>-1</sup> ]			
$V_0$ [L kg <sup>-1</sup> ]			
Solubility [g/mL]	Only slightly soluble in water <sup>[4]</sup> , readily dissolved in concentrated mineral acid from which it may be reprecipitated unchanged on dilution with water <sup>[4]</sup>		
Visible absorption maxima	Water: $\lambda_{\text{max}} = 428 \text{ m}\mu$ , $\epsilon_{\text{max}} = 1340$ , $\log \epsilon_{\text{max}} = 3.12$ <sup>[4]</sup> , dioxane: $\lambda_{\text{max}} = 428 \text{ m}\mu$ , $\epsilon_{\text{max}} = 1980$ , $\log \epsilon_{\text{max}} = 3.30$ <sup>[4]</sup>		

	Diaminotetrazine <sup>[1]</sup>	Diaminotetrazine <sup>[2]</sup>	Diaminotetrazine <sup>[3]</sup>
Chemical formula	C <sub>2</sub> H <sub>4</sub> N <sub>6</sub>	C <sub>2</sub> H <sub>4</sub> N <sub>6</sub>	C <sub>2</sub> H <sub>4</sub> N <sub>6</sub>
Molecular weight [g mol <sup>-1</sup> ]	112.1	112.1	112.1
Crystal system	Monoclinic	Orthorhombic	Orthorhombic
Space group	<i>C2/m</i>	<i>Amam</i> (no. 63)	<i>Cmcm</i>
<i>a</i> [Å]		6.257(1)	9.431(4)
<i>b</i> [Å]		7.839(1)	7.850(3)
<i>c</i> [Å]		9.424(1)	6.267(3)
$\alpha$ [°]		90	90
$\beta$ [°]		90	90
$\gamma$ [°]		90	90
<i>V</i> [Å <sup>3</sup> ]		462.234	464(3)
<i>Z</i>	2	4	8
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.624	1.611	1.605
<i>T</i> [K]		295	
	Recryst. from DMF	Brown crystals	

Orange-red microcrystalline solid on recryst. from dioxane and from water.<sup>[5]</sup>

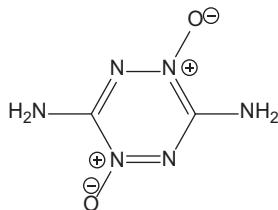
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### 3,6-Diamino-1,2,4,5-tetrazine-1,4-dioxide

Name [German, acronym]: 3-Amino-6-imino-4-oxido-1-oxo-5,6-dihydro-1*H*-1,2,4,5-tetrazin-1-ium-2-ide [LAX-112, DATZO<sub>2</sub>]

Main (potential) use: Extensively evaluated for use as an explosive<sup>[1]</sup>, extensively evaluated as an insensitive explosive<sup>[3]</sup>, considered as a fuel for digital microthrusters<sup>[3]</sup>, investigated as low-sensitivity explosive<sup>[6]</sup>

Structural formula:



	LAX-112
Formula	C <sub>2</sub> H <sub>4</sub> N <sub>6</sub> O <sub>2</sub>
Molecular mass [g mol <sup>-1</sup> ]	144.09
Appearance at RT	Reddish-brown crystals <sup>[6]</sup>
IS [J]	$H_{50} = 179 \text{ cm}$ (2.5 kg mass) <sup>[6]</sup> , 56% (cluster crystals (SEM), WL-1-type drop hammer, 1,000 ± 10 g, 250 ± 1 mm drop height, 50 mg sample) <sup>[6]</sup> , 12% (sheet crystals (SEM), WL-1-type drop hammer, 1,000 ± 10 g, 250 ± 1 mm drop height, 50 mg sample) <sup>[6]</sup>
FS [N]	Insensitive to friction <sup>[2]</sup> , 28% (cluster crystals (SEM), WM-1-type apparatus, 1,500 ± 1.5 g hammer weight, swing angle = 90 °, gauge pressure = 4 MPa, sliding column moving distance = 1.5–2.0 mm, 20 mg sample) <sup>[6]</sup> , 84% (cluster crystals (SEM), WM-1-type apparatus, 1,500 ± 1.5 g hammer weight, swing angle = 90 °, gauge pressure = 4 MPa, sliding column moving distance = 1.5–2.0 mm, 20 mg sample) <sup>[6]</sup>
N [%]	58.32
$\Omega(\text{CO}_2)$ [%]	-44.4
$T_{\text{m.p.}}$ [°C]	No mpt. <sup>[6]</sup>
$T_{\text{dec.}}$ [°C]	220 (exo, DSC) <sup>[3]</sup> , 266 (exo, DSC) <sup>[3]</sup> , 223–225 (onset), 275–277 (peak max) (DSC) <sup>[6]</sup> , 265.2 (peak, DSC @ 2 K/min) <sup>[6]</sup> , 277.7 (peak, DSC @ 5 K/min) <sup>[6]</sup> , 287.0 (peak, DSC @ 10 K/min) <sup>[6]</sup>

$\rho$ [g cm <sup>-3</sup> ]	1.86 (crystal) <sup>[2]</sup> , 1.85 (pressed) <sup>[3]</sup> , 1.834 <sup>[5,6]</sup>								
Heat of formation	39 kcal/mol <sup>[2]</sup> , 48 kcal/mol ( $\Delta_f H^\circ$ ) <sup>[3]</sup> , 164 kJ/mol (enthalpy of form.) <sup>[5,6]</sup>								
	Calcd. (EXPLO5 6.03)	Lit. values		Exptl.					
$-\Delta_{\text{ex}} U^\circ$ [kJ kg <sup>-1</sup> ]									
$T_{\text{ex}}$ [K]									
$p_{\text{C-J}}$ [kbar]			25.7 GPa (@ 1.615 g cm <sup>-3</sup> , calcd.) <sup>[5]</sup>	30.1 ( $\rho$ not specified, 95:5 mixture of LAX-112/Viton A) <sup>[2]</sup>					
VoD [m s <sup>-1</sup> ]			8,786 (@ 1.88 g cm <sup>-3</sup> , calcd.) <sup>[3]</sup>  $\approx$ 8,300 (@ unspecified $\rho$ ) <sup>[4]</sup>  7,790 (@ 1.615 g cm <sup>-3</sup> , calcd.) <sup>[5]</sup>	8,100 ( $\rho$ not specified, 95:5 mixture of LAX-112/Viton A) <sup>[2]</sup>					
$V_0$ [L kg <sup>-1</sup> ]									
Critical diameter [cm]	<6 mm <sup>[5,6]</sup>								
Thermal stability	Thermally stable up to 206 °C <sup>[2]</sup>								
Solubility [g/mL]	Recryst. from DMSO/H <sub>2</sub> O <sup>[6]</sup>								
Compatibility	Can be formulated with binders such as Kel-F or Viton A <sup>[2]</sup>								
Wedge test	95% LAX-112/5% OXY 461, molding powder pressed @ 42,000 psi and 110 °C to achieve ~97.8% of the 1.829 g/cc formulation TMD <sup>[4]</sup> :								
	$\rho_0$ (g/cm <sup>3</sup> )	$p_0$ (GPa)	$u_p$ (km/s)	$U_s$ (km/s)	$x^*$ (mm)				
	1.793	7.5	0.95	4.41	8.00				
	1.794 10.4	1.19	4.86	5.06	0.99				
	1.794	13.7	1.41	5.43	2.12				
	1.793	22.2	1.84	6.74	0.74				
					0.36				
					0.12				

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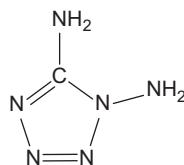
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## 1,5-Diamino-1,2,3,4-tetrazole

Name [German, acronym]: Diaminotetrazole, 1,5-diaminotetrazole  
 [1,5-diaminotetrazol, diaminotetrazol, DAT]

Main (potential) use: Starting material for synthesis of other energetic materials<sup>[9]</sup>, possible gas-generating agent<sup>[7]</sup>, possible blowing agent for polymeric systems<sup>[7]</sup>, possible materials for gas-generating compositions<sup>[10]</sup>

Structural formula:



	DAT
Formula	CH <sub>4</sub> N <sub>6</sub>
Molecular mass [g mol <sup>-1</sup> ]	100.09
Appearance at RT	Colorless crystals (prisms) <sup>[2]</sup> , crystalline <sup>[4]</sup> , white crystals <sup>[9]</sup>
IS [J]	
FS [N]	
ESD [J]	
N [%]	83.97
Ω(CO <sub>2</sub> ) [%]	-63.9
T <sub>m.p.</sub> [°C]	185–187 <sup>[3]</sup> , 460 K <sup>[4,6]</sup> , 187 (endo, peak max, DSC @ 10 K/min, 60 mL/min N <sub>2</sub> flow) <sup>[6]</sup> , 459 K (DAT recryst. from H <sub>2</sub> O) <sup>[7]</sup> , 460 K (DSC @ 10 K/min, inert gas flow) <sup>[7]</sup> , 460 K (DSC @ 10 K/min, @ elevated pressure in inert atmosphere) <sup>[7]</sup> , 460 K (DSC @ 10 K/min, sealed crucible in self-generated atmosphere) <sup>[7]</sup> , 186–187 (crystals) <sup>[9]</sup> , 186–187 <sup>[10,11]</sup> , 186 <sup>[11]</sup>
T <sub>phase transition</sub> [°C]	~493 K (calcd. X-ray powder diffraction pattern) <sup>[5]</sup>
T <sub>dec.</sub> [°C]	470–620 K (one main step dec., followed by slow weight loss until 870 K, 85% mass loss) <sup>[4,6]</sup> , 470–540 K (DSC @ 10 K/min, inert gas flow) <sup>[7]</sup> , 470–540 K (DSC @ 10 K/min, @ elevated pressure in inert atmosphere) <sup>[7]</sup> , 470–540 K (DSC @ 10 K/min, sealed crucible in self-generated atmosphere) <sup>[7]</sup> , 470–540 K (~85% weight loss, @ 10 K/min, N <sub>2</sub> flow of 60 mL/min), 187–188 <sup>[12]</sup>
ρ [g cm <sup>-3</sup> ]	1.571 (crystal) <sup>[2]</sup> , 1.735 (crystal) <sup>[10]</sup>

Heat of formation	$74.18 \pm 0.24$ kJ/mol ( $\Delta H_f^\circ$ , exptl. from measured enthalpies of combustion using calorimeter) <sup>[1,11]</sup> , $74.5 \pm 1.5$ kcal/mol ( $\Delta_f H^\circ$ solid) <sup>[4,10]</sup> , $100.7 \pm 1.0$ kcal/mol ( $\Delta_f H^\circ$ gas) <sup>[4]</sup> , 3,891 kJ/kg (gas phase) <sup>[8]</sup>		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{\text{ex}} U^\circ$ [kJ kg <sup>-1</sup> ]			
$T_{\text{ex}}$ [K]			
$p_{\text{C}_j}$ [kbar]			
VoD [m s <sup>-1</sup> ]			
$V_0$ [L kg <sup>-1</sup> ]			
Burn rate [mm/s]	Only starts to burn at extremely high pressures (>24 MPa) <sup>[10]</sup> , does not sustain stable combustion @ pressures <20 MPa <sup>[10]</sup> , 21 mm/s @ 30 MPa <sup>[10,11]</sup> , ~ 6 mm/s @ 25 MPa <sup>[10]</sup> , ~ 15 mm/s @ 28 MPa <sup>[10]</sup> , ~ 25 mm/s @ 35 MPa <sup>[10]</sup> , no burning observed @ 10 MPa pressure, only achieves steady-state combustion >30 MPa (pressed cylinder sample @ 0.90–0.94 TMD, 7 mm diameter) <sup>[11]</sup>		
Solubility [g/mL]	Soluble in hot EtOH <sup>[3]</sup> , recryst. from H <sub>2</sub> O <sup>[2,3,7,12]</sup> , readily soluble in hot water, aqueous alcoholic mixtures, acids and DMFA <sup>[9]</sup> , moderately soluble in cold water, EtOH <sup>[9]</sup> , insoluble in THF, ethyl acetate, methylene chloride, Et <sub>2</sub> O <sup>[9]</sup> , soluble in ethyl acetate <sup>[12]</sup>		
$\Delta H^\circ_{\text{sol}}$ [kJ/mol]	$7.66 \pm 0.03$ (@ 298 K) <sup>[1]</sup>		
$\Delta_{\text{subl.}} H^\circ$ [kcal/mol]	$26.2 \pm 0.5$ <sup>[4]</sup>		
$\Delta H_{\text{dec}}$ [kJ mol <sup>-1</sup> ]	850 (DSC @ 10 K/min, 10 atm N <sub>2</sub> pressure) <sup>[6]</sup>		
Compatibility	Reacts with strong acids as monohydric base forming the corresponding salt <sup>[9]</sup> , readily reacts with carbonyl compounds <sup>[9]</sup> , forms stable complex with copper(II) chloride <sup>[9]</sup>		
Adiabatic flame $T$ [K]	2,087 <sup>[10,11]</sup>		

	1,5-Diaminotetrazole <sup>[2]</sup>	1,5-Diaminotetrazole <sup>[5]</sup>
Chemical formula	CH <sub>4</sub> N <sub>6</sub>	CH <sub>4</sub> N <sub>6</sub>
Molecular weight [g mol <sup>-1</sup> ]	100.10	100.10
Crystal system	Monoclinic	Monoclinic
Space group	P2 <sub>1</sub> /c	P2 <sub>1</sub> /c
$a$ [\AA]	6.7800(10)	6.392

<i>b</i> [Å]	6.1120(10)	7.277
<i>c</i> [Å]	10.694(2)	9.803
$\alpha$ [°]	90	90
$\beta$ [°]	107.250(10)	90.24
$\gamma$ [°]	90	90
<i>V</i> [Å <sup>3</sup> ]	423.20(10)	
<i>Z</i>	4	
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.571	
<i>T</i> [K]	293	
	Colorless prisms	Powder X-ray diffraction

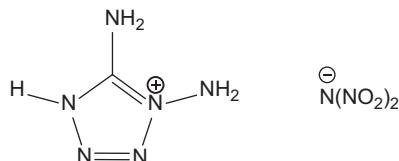
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## 1,5-Diaminotetrazolium dinitramide

Name [German, acronym]: Diaminotetrazoliumdinitramide,  
 [1,5-diaminotetrazolium dinitramid, HDAT-DN]

Main (potential) use: oxidizer

Structural formula:



	HDAT-DN		
Formula	$\text{CH}_5\text{N}_9\text{O}_4$		
Molecular mass [g mol <sup>-1</sup> ]	207.11		
Appearance at RT	Colorless crystals <sup>[1]</sup>		
IS [J]	2 (75–125 µm particle size, BAM) <sup>[1]</sup>		
FS [N]	5 (75–125 µm particle size, BAM) <sup>[1]</sup>		
ESD [J]	670 mJ (OZM apparatus) <sup>[1]</sup>		
N [%]	60.87		
$\Omega(\text{CO}_2)$ [%]	-3.9		
$T_{\text{m.p.}}$ [°C]	135 (dec. without melting, DSC @ 5 K/min, pressed Al containers with hole) <sup>[1]</sup>		
$T_{\text{dec.}}$ [°C]	135 (dec. without melting, DSC @ 5 K/min, pressed Al containers with hole) <sup>[1]</sup>		
$\rho$ [g cm <sup>-3</sup> ]	1.771 (X-ray @ 200 K) <sup>[1]</sup>		
Heat of formation	431 kJ/mol ( $\Delta H_f^\circ$ ) <sup>[1,2]</sup> , 97.7 kcal/mol ( $\Delta_f H^\circ$ (s)) <sup>[1]</sup>		
	Calcd. (EXPLO5 5.02)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^\circ$ [kJ kg <sup>-1</sup> ]	6,192 <sup>[1,2]</sup>		
$T_{\text{ex}}$ [K]	4,632 <sup>[1]</sup>		
$p_{\text{CJ}}$ [kbar]	360 <sup>[1,2]</sup>		
VoD [m s <sup>-1</sup> ]	9,306 (@ 1.771 g cm <sup>-3</sup> ) <sup>[1,2]</sup>		
$V_0$ [L kg <sup>-1</sup> ]	865 <sup>[1]</sup>		

	<b>1,5-Diaminotetrazolium dinitramide<sup>[1]</sup></b>
Chemical formula	$\text{CH}_5\text{N}_9\text{O}_4$
Molecular weight [g mol <sup>-1</sup> ]	207.14
Crystal system	Monoclinic
Space group	$P2_1/c$ (no. 14)
<i>a</i> [\AA]	15.7942(8)
<i>b</i> [\AA]	10.1115(4)
<i>c</i> [\AA]	10.2757(5)
$\alpha$ [°]	90
$\beta$ [°]	108.817(6)
$\gamma$ [°]	90
<i>V</i> [\AA <sup>3</sup> ]	1,553.35(14)
<i>Z</i>	8
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.771
<i>T</i> [K]	200
	Colorless crystals from EtOH

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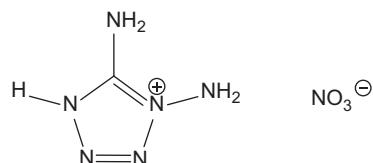
[2] T. M. Klapötke, J. Stierstorfer, *Eur. J. Inorg. Chem.*, **2008**, 4055–4062.

## 1,5-Diamino-1*H*-tetrazolium nitrate

Name [German, acronym]: Diaminotetrazoliumnitrate, 1,5-diaminotetrazole nitrate  
[diaminotetrazolium nitrat, DAT\_N]

Main (potential) use: explosive

Structural formula:



	DAT-N		
Formula	$\text{CH}_5\text{N}_7\text{O}_3$		
Molecular mass [g mol <sup>-1</sup> ]	163.10		
Appearance at RT	White crystals <sup>[4]</sup> , colorless plates <sup>[5]</sup>		
IS [J]	9 (BAM, 20 mg sample) <sup>[5]</sup>		
FS [N]	192 (BAM) <sup>[5]</sup>		
N [%]	60.12		
$\Omega(\text{CO}_2)$ [%]	-14.7		
$T_{\text{m.p.}}$ [°C]	136–138 (dec.) <sup>[4]</sup> , 138 (DSC @ 10 °C/min) <sup>[5]</sup>		
$T_{\text{dec.}}$ [°C]	168 (DSC @ 10 °C/min) <sup>[1,5]</sup> , 193 ± 14 (onset dec, T, MS @ 326,000 K/s; 0.5 ms reaction time) <sup>[1]</sup> , 583 K (0.5 ms reaction time, MS @ 560,000 K/s) <sup>[3]</sup>		
$\rho$ [g cm <sup>-3</sup> ]	1.727 (X-ray, crystal @ 293 K) <sup>[5]</sup>		
Heat of formation	60.7 kcal/mol ( $\Delta_f H^\circ$ , calcd., G2 method) <sup>[5]</sup>		
Heat of combustion	-1,993 cal/g (calcd.) <sup>[5]</sup> , -1,888 cal/g (exptl.) <sup>[5]</sup>		
Calcd. (EXPLO5 6.04)	Lit. values	Exptl.	
$-\Delta_{\text{ex}}U^\circ$ [kJ kg <sup>-1</sup> ]		$-\Delta_{\text{ex}}H = 1,245$ cal/g (calcd.) <sup>[5]</sup>	
$T_{\text{ex}}$ [K]			
$p_{\text{C-J}}$ [kbar]		33.3 GPa (calcd., K-J) <sup>[5]</sup>	
VoD [m s <sup>-1</sup> ]		8,774 (@ 1.727 g cm <sup>-3</sup> , calcd., K-J) <sup>[5]</sup>	

$V_0$ [L kg <sup>-1</sup> ]			
Solubility [g/mL]	Soluble in H <sub>2</sub> O <sup>[4,5]</sup>		

	HDAT-NO <sub>3</sub> <sup>[2,5]</sup>
Chemical formula	CH <sub>5</sub> N <sub>7</sub> O <sub>3</sub>
Molecular weight [g mol <sup>-1</sup> ]	163.12
Crystal system	Monoclinic
Space group	C2/c (no. 25)
<i>a</i> [\AA]	17.898(3)
<i>b</i> [\AA]	5.2292(8)
<i>c</i> [\AA]	14.479(2)
$\alpha$ [°]	90
$\beta$ [°]	112.23(1)
$\gamma$ [°]	90
<i>V</i> [\AA <sup>3</sup> ]	1,254.3(3)
<i>Z</i>	8
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.727
<i>T</i> [K]	293

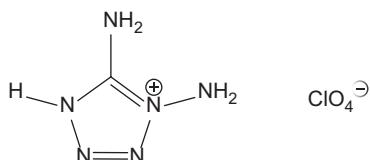
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- [4] P. N. Gaponik, V. P. Karavai, *Chem. Heterocycl. Compounds*, **1984**, *20*, 1388–1391.
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## 1,5-Diamino-1*H*-tetrazolium perchlorate

Name [German, acronym]: Diaminotetrazoliumperchlorate,  
1,5-diaminotetrazolium perchlorate  
[1,5-diaminotetrazolium perchlorat, DAT•HClO<sub>4</sub>]

Main (potential) use: oxidizer

Structural formula:



	DAT•HClO <sub>4</sub>		
Formula	CH <sub>5</sub> CIN <sub>6</sub> O <sub>4</sub>		
Molecular mass [g mol <sup>-1</sup> ]	200.54		
Appearance at RT	White crystals <sup>[1,2]</sup> , large colorless plates <sup>[3]</sup> , highly crystalline solid <sup>[4]</sup> , chunky crystals <sup>[4]</sup>		
IS [J]	7 (20 mg sample, BAM) <sup>[3]</sup> , sensitive to hammer blow <sup>[4]</sup>		
FS [N]	60 (BAM) <sup>[3]</sup>		
N [%]	41.9		
Ω(CO <sub>2</sub> ) [%]	-5.5		
T <sub>m.p.</sub> [°C]	113–114 <sup>[1,2]</sup> , 97–98 <sup>[1,2]</sup> , 125–130 <sup>[1,2,4]</sup> , 97 (DSC @ 10 °C/min) <sup>[3]</sup>		
T <sub>dec.</sub> [°C]	192 (peak max, DSC @ 10 °C/min) <sup>[3]</sup>		
ρ [g cm <sup>-3</sup> ]	1.090 (single crystal) <sup>[2]</sup>		
Heat of formation	28 kcal/mol (enthalpy of form., calcd.) <sup>[1]</sup> , 35.5 kcal/mol (enthalpy of form.) <sup>[2]</sup> , 45.9 kcal/mol (ΔH <sub>f</sub> <sup>o</sup> , calcd., G2 method) <sup>[3]</sup>		
Heat of combustion	-972 cal/g (Δ <sub>c</sub> H, exptl. molar enthalpy of combustion) <sup>[3]</sup> , -199 kcal/mol (Δ <sub>c</sub> U, exptl. constant vol. combustion energy) <sup>[3]</sup>		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
-Δ <sub>ex</sub> U <sup>o</sup> [kJ kg <sup>-1</sup> ]		Δ <sub>E</sub> H = 928 cal/g (calcd. molar enthalpy of detonation) <sup>[3]</sup>	
T <sub>ex</sub> [K]			

$p_{C,J}$ [kbar]			
VoD [ $\text{m s}^{-1}$ ]			
$V_0$ [ $\text{L kg}^{-1}$ ]			
5 s explosion $T$ [ $^{\circ}\text{C}$ ] Ignition $T$ [ $^{\circ}\text{C}$ ]	192 <sup>[1]</sup>		
Burn rate [mm/s]	149 @ 10 MPa (pressed cylinder sample @ 0.90–0.94 TMD, 7 mm diameter) <sup>[1]</sup> , 18 @ 0.1 MPa <sup>[1,2]</sup> , 30 @ 0.35 MPa <sup>[1,2]</sup> , 40 @ 0.6 MPa <sup>[1,2]</sup> , 49 @ 0.9 MPa <sup>[1,2]</sup> , 65 @ 2 MPa <sup>[1,2]</sup> , 90 @ 4 MPa <sup>[1,2]</sup> , 120 @ 6.5 MPa <sup>[1,2]</sup> , 180 @ 10 MPa <sup>[2]</sup>		
Solubility [g/mL]	Soluble in a wide range of polar solvents such as $\text{CH}_3\text{CN}$ , water, EtOH, MeOH, DMSO and DMF <sup>[4]</sup>		
Adiabatic flame $T$ [ $^{\circ}\text{C}$ ]	3,285 <sup>[1]</sup> , 3,325 <sup>[2]</sup>		
Flash $T$ [ $^{\circ}\text{C}$ ]	192 <sup>[2]</sup>		

	DAT• $\text{HClO}_4$ <sup>[3]</sup>	DAT• $\text{HClO}_4$ <sup>[4]</sup>
Chemical formula	$\text{CH}_5\text{ClN}_6\text{O}_4$	$\text{CH}_5\text{ClN}_6\text{O}_4$
Molecular weight [g mol <sup>-1</sup> ]	200.56	200.56
Crystal system	Monoclinic	Monoclinic
Space group	$C2/c$	$P2_1/n$ (no. 14)
$a$ [\mathring{A}]	9.063(3)	9.0683(8)
$b$ [\mathring{A}]	5.013(1)	4.9956(4)
$c$ [\mathring{A}]	15.659(4)	15.636(1)
$\alpha$ [°]	90	90
$\beta$ [°]	100.022(5)	99.857(2)
$\gamma$ [°]	90	90
$V$ [\mathring{A} <sup>3</sup> ]	700.5(4)	697.9(1)
$Z$	4	4
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.902	1.909
$T$ [K]	193	100

[1] V. P. Sinditskii, V. Y. Egorshev, M. D. Dutova, T. Y. Dutov, *Combustion of 1,5-Diaminotetrazole Derivatives*, in *Theory and Practice of Energetic Materials* (vol. VIII): Proc. 2009 Int. Autumn Seminar on Propellants, Explosives and Pyrotechnics, Kunming, China, 22nd–25th September 2009, S. Li, Y. Wang, F. Cao, S. Zhao, S. Zhou, Science Press.

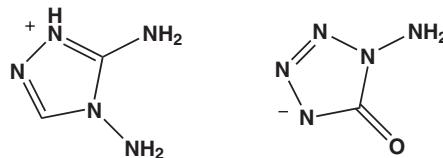
- [2] V. P. Sinditskii, V. Y. Egorshev, T. Y. Dutov, M. D. Dutova, T. -L. Zhang, J. -G. Zhang, *Combust., Explosion, Shock Waves*, **2011**, *47*, 36–44.
- [3] J. C. Gálvez-Ruiz, G. Holl, K. Karaghiosoff, T. M. Klapötke, K. Löhnwitz, P. Mayer, H. Nöth, K. Polborn, C. J. Rohbogner, M. Suter, J. J. Weigand, *Inorg. Chem.*, **2005**, *44*, 4237–4253.
- [4] G. Drake, T. Hawkings, L. Hall, J. Boatz, A. Vij, *Experimental and Theoretical Study of 1,5-Diamino-1,2,3,4-Tetrazolium Perchlorate, Propellants, Explosives, Pyrotechnics*, AFRL-PR-ED-TP-2004-119, Air Force Research Laboratory, Edwards Air Force Base, California, USA, April **2005**.

## 3,4-Diamino-1,2,4-triazolium 1-aminotetrazol-5-oneate

Name [German, acronym]: 3,4-Diamino-1,2,4-triazolium 1-aminotetrazol-5-oneate  
[ATO · DATr]

Main (potential) use: Secondary (high) explosive

Structural formula:



	ATO · DATr
Formula	C <sub>3</sub> H <sub>8</sub> N <sub>10</sub> O
Molecular mass [g mol <sup>-1</sup> ]	200.19
Appearance at RT	White powder <sup>[1]</sup>
IS [J]	>40 <sup>[1]</sup>
N [%]	68.98
Ω(CO <sub>2</sub> ) [%]	-48.0
T <sub>m.p.</sub> [°C]	170.0 (DSC-TG @ 10 °C/min) <sup>[1]</sup>
T <sub>dec.</sub> [°C]	220.5 (DSC-TG @ 10 °C/min) <sup>[1]</sup>
ρ [g cm <sup>-3</sup> ]	1.632 (@ 298 K) <sup>[1]</sup>
Heat of formation	494.36 kJ/mol ( $\Delta_f H^\circ$ , calcd.) <sup>[1]</sup> , 2,471.8 kJ kg <sup>-1</sup> ( $\Delta_f H^\circ$ , calcd.) <sup>[1]</sup>
	Calcd. (K-J)
	Exptl.
-Δ <sub>ex</sub> U <sup>o</sup> [kJ kg <sup>-1</sup> ]	
T <sub>ex</sub> [K]	
p <sub>C-J</sub> [kbar]	23.6 <sup>[1]</sup>
VoD [m s <sup>-1</sup> ]	7,530 <sup>[1]</sup>
V <sub>0</sub> [L kg <sup>-1</sup> ]	

	ATO-DATr <sup>[1]</sup>
Chemical formula	C <sub>3</sub> H <sub>8</sub> N <sub>10</sub> O
Molecular weight [g mol <sup>-1</sup> ]	200.19
Crystal system	Triclinic

Space group	P-1 (no. 2)
$a$ [Å]	6.0700(6)
$b$ [Å]	7.1682(7)
$c$ [Å]	10.6018(9)
$\alpha$ [°]	76.5820(10)
$\beta$ [°]	88.343(2)
$\gamma$ [°]	65.4060(10)
$V$ [Å <sup>3</sup> ]	407.32(7)
$Z$	2
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.632
$T$ [K]	298

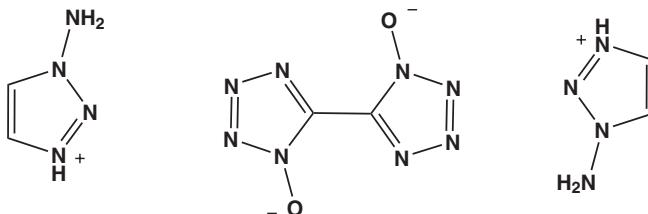
- [1] X. Yin, J. -T. Wu, X. Jin, C. -X. Xu, P. He, T. Li, K. Wang, J. Qin, J. -G. Zhang, *RSC Adv.*, **2015**, *5*, 60005–60014.

**Di(1-amino-1,2,3-triazolium) 5,5'-bitetrazole-1,1'-diolate**

Name [German, acronym]: Di(1-amino-1,2,3-triazolium) 5,5'-bitetrazole-1,1'-diolate  
[2ATr · BTO]

Main (potential) use: Secondary explosive

Structural formula:



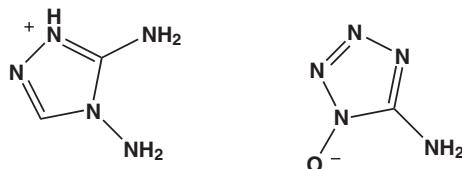
<b>2ATr.BTO</b>		
Formula	$C_6H_{10}N_{16}O_2$ , $[C_2H_5N_4]^+ \cdot [C_2N_8O_2]^{2-}$	
Molecular mass [g mol <sup>-1</sup> ]	345.21	
Appearance at RT		
IS [J]	32	
N [%]	66.2	
$\Omega(CO_2)$ [%]	-70.9	
$T_{dec.}$ [°C]	247 (DSC @ 5 °C/min)	
$\rho$ [g cm <sup>-3</sup> ]	1.691 (@ 298 K)	
Heat of formation	1,273.6 kJ/mol ( $\Delta_f H^\circ$ )	
	Calcd. (K-J)	Exptl.
$-\Delta_{ex}U^\circ$ [kJ kg <sup>-1</sup> ]		
$T_{ex}$ [K]		
$p_{C_J}$ [kbar]	272	
VoD [m s <sup>-1</sup> ]	7,957	
$V_0$ [L kg <sup>-1</sup> ]		

## 3,4-Diamino-1,2,4-triazolium 1-hydroxyl-5-amino-tetrazolate

Name [German, acronym]: 3,4-Diamino-1,2,4-triazolium 1-hydroxyl-5-amino-tetrazolate [DATr.HATZ]

Main (potential) use: Secondary explosive

Structural formula:



	DATr.HATZ
Formula	C <sub>3</sub> H <sub>8</sub> N <sub>10</sub> O, [C <sub>2</sub> H <sub>6</sub> N <sub>5</sub> ] <sup>+</sup> [CH <sub>2</sub> N <sub>5</sub> O] <sup>-</sup>
Molecular mass [g mol <sup>-1</sup> ]	200.09
Appearance at RT	
IS [J]	38 <sup>[1]</sup>
N [%]	56.4
Ω(CO <sub>2</sub> ) [%]	-44.0
T <sub>m.p.</sub> [°C]	195 <sup>[1]</sup>
T <sub>dec.</sub> [°C]	225 (DSC @ 5 °C/min) <sup>[1]</sup>
ρ [g cm <sup>-3</sup> ]	1.692 (@ 296 K)
Heat of formation	571.9 kJ/mol (Δ <sub>f</sub> H <sup>o</sup> ) <sup>[1]</sup>
	Calcd. (K-J)
	Exptl.
-Δ <sub>ex</sub> U <sup>o</sup> [kJ kg <sup>-1</sup> ]	
T <sub>ex</sub> [K]	
p <sub>C-J</sub> [kbar]	264 <sup>[1]</sup>
VoD [m s <sup>-1</sup> ]	7,856 <sup>[1]</sup>
V <sub>0</sub> [L kg <sup>-1</sup> ]	

	DATr-HATZ <sup>[1]</sup>
Chemical formula	C <sub>3</sub> H <sub>8</sub> N <sub>10</sub> O
Molecular weight [g mol <sup>-1</sup> ]	200.19
Crystal system	Triclinic
Space group	P-1 (no. 2)
<i>a</i> [Å]	6.0700(6)
<i>b</i> [Å]	7.1682(7)
<i>c</i> [Å]	10.6018(9)
$\alpha$ [°]	76.8520(10)
$\beta$ [°]	88.343(2)
$\gamma$ [°]	65.4060(10)
<i>V</i> [Å <sup>3</sup> ]	407.32(7)
<i>Z</i>	2
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.632
<i>T</i> [K]	298

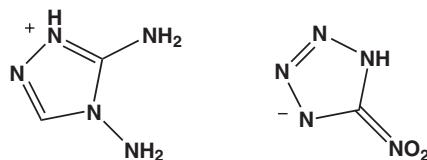
[1] X. Yin, J.-T. Wu, X. Jin, C.-X. Xu, P. He, T. Li, K. Wang, J. Qin, J.-G. Zhang, *RSC Adv.*, **2015**, *5*, 60005–60014.

### 3,4-Diamino-1,2,4-triazolium 5-nitramino-tetrazolate

Name [German, acronym]: 3,4-Diamino-1,2,4-triazolium 5-nitramino-tetrazolate  
 [DATr.NATZ]

Main (potential) use: Secondary explosive

Structural formula:



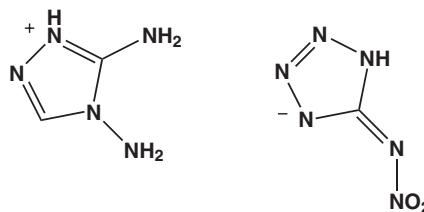
	DATr.NATZ
Formula	C <sub>3</sub> H <sub>7</sub> N <sub>11</sub> O <sub>2</sub> , [C <sub>2</sub> H <sub>6</sub> N <sub>5</sub> ] <sup>+</sup> [CHN <sub>6</sub> O <sub>2</sub> ] <sup>-</sup>
Molecular mass [g mol <sup>-1</sup> ]	220.08
Appearance at RT	
IS [J]	6.5
N [%]	67.2
Ω(CO <sub>2</sub> ) [%]	-52.4
T <sub>m.p.</sub> [°C]	196
T <sub>dec.</sub> [°C]	204 (DSC @ 5 °C/min)
ρ [g cm <sup>-3</sup> ]	1.661 (@ 296 K)
Heat of formation	484 kJ/mol (Δ <sub>f</sub> H°)
	Calcd. (K-J)
	Exptl.
-Δ <sub>ex</sub> U° [kJ kg <sup>-1</sup> ]	
T <sub>ex</sub> [K]	
p <sub>C-J</sub> [kbar]	256
VoD [m s <sup>-1</sup> ]	7,789
V <sub>0</sub> [L kg <sup>-1</sup> ]	

**3,4-Diamino-1,2,4-triazolium 5-nitro-tetrazolate**

Name [German, acronym]: Di(3,4-diamino-1,2,4-triazolium) 5-dinitromethyl-tetrazolate [DATr.NTZ]

Main (potential) use: Secondary explosive

Structural formula:



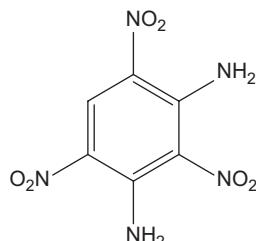
	DATr.NTZ	
Formula	C <sub>3</sub> H <sub>6</sub> N <sub>10</sub> O <sub>2</sub> , [C <sub>2</sub> H <sub>6</sub> N <sub>5</sub> ] <sup>+</sup> [CN <sub>5</sub> O <sub>2</sub> ] <sup>-</sup>	
Molecular mass [g mol <sup>-1</sup> ]	214.07	
Appearance at RT		
IS [J]	11	
N [%]	65.4	
Ω(CO <sub>2</sub> ) [%]	-52.3	
T <sub>m.p.</sub> [°C]	140	
T <sub>dec.</sub> [°C]	247 (DSC @ 5 °C/min)	
ρ [g cm <sup>-3</sup> ]	1.739 (@ 298 K)	
Heat of formation	484 kJ/mol (Δ <sub>f</sub> H°)	
	Calcd. (K-J)	Exptl.
-Δ <sub>ex</sub> U° [kJ kg <sup>-1</sup> ]		
T <sub>ex</sub> [K]		
p <sub>C-J</sub> [kbar]	271	
VoD [m s <sup>-1</sup> ]	7,892	
V <sub>0</sub> [L kg <sup>-1</sup> ]		

## Diaminotnitrobenzene

Name [German, acronym]: Diaminotnitrobenzene, 2,4,6-trinitro-1,3-diaminobenzene, trinitro-*m*-phenylenediamine, [diaminotnitrobenzol, 2,4,6-trinitro-1,3-diaminobenzol, DATB, DATNB]

Main (potential) use: Pressed explosive or ballistic modifier in some rocket propellants<sup>[2]</sup>, temperature-resistant high explosive, special applications in warheads of high speed guided missiles<sup>[39]</sup>, relatively insensitive, temperature-resistant high explosive which is only effectively used in military applications if coated with plastic or mixed with liquid components<sup>[3]</sup>

Structural formula:



	<b>DATB</b>
Formula	$\text{C}_6\text{H}_5\text{N}_5\text{O}_6$
Molecular mass [g mol <sup>-1</sup> ]	243.14
Appearance at RT	Yellow crystalline solid <sup>[2,3,39,42]</sup> , yellow needles <sup>[42]</sup> , lemon yellow crystalline substance <sup>[47]</sup>
IS [J]	200% TNT <sup>[2]</sup> , $H_{50} > 320 \text{ cm}$ (tool type 12) <sup>[3]</sup> , $H_{50} = 230 \text{ cm}$ (tool type 12B) <sup>[3]</sup> , $H_{50} = 320 \text{ cm}$ <sup>[6,12,16]</sup> , $H_0 > 177 \text{ cm}$ (tool type 12, 5 kg mass) <sup>[7]</sup> , $H_{50} > 177 \text{ cm}$ (tool type 12B, 5 kg mass) <sup>[7]</sup> , $H_{50} > 111.6$ <sup>[8]</sup> , $H_{50\%} > 200 \text{ cm}$ (B.M., type 12 tool, 2.5 kg mass, 35 mg sample, garnet paper) <sup>[22]</sup> , 20.6 in (burned, no explosion, P.A.) <sup>[14]</sup> , $> 60 \text{ cm}$ (max. fall for $\frac{1}{6}$ shots, 2 kg mass, Lenze-Kast app.) <sup>[11]</sup> , $> 24 \text{ cm}$ (max. fall for $\frac{1}{6}$ shots, 10 kg mass, Lenze-Kast app.) <sup>[11]</sup> , $> 60 \text{ cm}$ (min. fall for $\frac{1}{6}$ shots, 10 kg mass, Lenze-Kast app.) <sup>[11]</sup> , $> 24 \text{ cm}$ (min. fall for $\frac{1}{6}$ shots, 10 kg mass, Lenze-Kast app.) <sup>[11]</sup> , 50% impact height $> 320 \text{ cm}$ <sup>[26]</sup> , $> 320 \text{ cm}$ (NEDED) <sup>[27]</sup> , $> 320 \text{ cm}$ (NOL) <sup>[27]</sup> , $> 320 \text{ cm}$ (LANL) <sup>[27]</sup> , less sensitive than tetryl but more sensitive than PA <sup>[28]</sup> , $H_{50} = 320 \text{ cm}$ (78.4 J) <sup>[29]</sup> , 320 cm (Bruceton method, type 12 tool, 2.5 kg mass, 40 mg sample, 5/0 sandpaper, 25 trials) <sup>[30]</sup> , 320 cm (2.5 kg mass) <sup>[33]</sup> , 150.7 cm (5 kg mass, AFATL) <sup>[33]</sup> ,

	<p><math>H_{50} = 320 \text{ cm}</math> (2.5 kg mass, type 12 tool)<sup>[36]</sup>, <math>\log(H_{50}) = 2.505</math> (Kamlet/Adolph)<sup>[37]</sup>, 35+ in (2 kg mass, confined, height of no detonation, P.A.)<sup>[43]</sup>, IS of form II (high <math>T</math> form) is the same as that of form I (ERL apparatus)<sup>[48]</sup>, <math>H_{50} = 320 \text{ cm}</math><sup>[54]</sup>, <math>H_{50\%} \geq 200 \text{ cm}</math> (2.5 kg mass, type 12 tool, 35 mg sample in conical pile, 1 in<sup>2</sup> garnet paper)<sup>[55]</sup>, <math>H_{50\%} = 320 \text{ cm}</math> (2.5 kg mass)<sup>[57]</sup></p> <p>ERL apparatus, data from ref.<sup>[3]</sup></p> <table border="1"> <thead> <tr> <th rowspan="2">Explosive</th> <th>Type 12</th> <th>Type 12B</th> </tr> <tr> <th><math>H_{50}</math> (cm)</th> <th><math>H_{50}</math> (cm)</th> </tr> </thead> <tbody> <tr> <td>96 DATB/5 Viton</td> <td>&gt;320</td> <td>&gt;320</td> </tr> <tr> <td>95 DATB/2.5 PS/2.5 DOP</td> <td>&gt;320</td> <td>&gt;320</td> </tr> <tr> <td>95 DATB/5 Estane</td> <td>&gt;320</td> <td>&gt;320</td> </tr> <tr> <td>95 DATB/5 Kel-F</td> <td>&gt;320</td> <td>&gt;320</td> </tr> </tbody> </table> <p>Rotter impact data: 27 mg sample, Bruceton method/25 drop run to obtain <math>H_{50\%}</math>; initiation criteria = 1 mL gas evolved or 0.5 mL accompanied by smoke or evidence of burning in the sample; data from ref.<sup>[52]</sup></p> <table border="1"> <thead> <tr> <th colspan="2">Rotter impact data</th> <th colspan="2">US data</th> </tr> <tr> <th>F of I</th> <th>Gas evolved (mL)</th> <th>NSWC/NOL, ERL type 12</th> <th>NWC B.M. type 12</th> </tr> </thead> <tbody> <tr> <td>170</td> <td>0.5</td> <td>320</td> <td>&gt;200</td> </tr> </tbody> </table> <p>IS for irradiated explosives, 50% fire height in inches, Bruceton method (P.A. apparatus, 2 kg mass)<sup>[56]</sup>:</p> <table border="1"> <thead> <tr> <th>Total Co<sup>60</sup> gamma dose (R)</th> <th>X mean (in)</th> <th><math>\sigma</math> std. dev. (in)</th> </tr> </thead> <tbody> <tr> <td>0</td> <td>20.64</td> <td>6.20</td> </tr> <tr> <td><math>1.5 \times 10^7</math></td> <td>19.00</td> <td>1.26</td> </tr> <tr> <td><math>1.3 \times 10^8</math></td> <td>17.80</td> <td>1.99</td> </tr> <tr> <td><math>1.2 \times 10^9</math></td> <td>13.50</td> <td>1.51</td> </tr> </tbody> </table>	Explosive	Type 12	Type 12B	$H_{50}$ (cm)	$H_{50}$ (cm)	96 DATB/5 Viton	>320	>320	95 DATB/2.5 PS/2.5 DOP	>320	>320	95 DATB/5 Estane	>320	>320	95 DATB/5 Kel-F	>320	>320	Rotter impact data		US data		F of I	Gas evolved (mL)	NSWC/NOL, ERL type 12	NWC B.M. type 12	170	0.5	320	>200	Total Co <sup>60</sup> gamma dose (R)	X mean (in)	$\sigma$ std. dev. (in)	0	20.64	6.20	$1.5 \times 10^7$	19.00	1.26	$1.3 \times 10^8$	17.80	1.99	$1.2 \times 10^9$	13.50	1.51
Explosive	Type 12		Type 12B																																										
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FS [N]	$F_{50} > 36 \text{ kgf}$ <sup>[8]</sup>																																												
ESD [J]	$E_{50} = 29.84$ (@ 293 K) <sup>[8]</sup> , $E_{50} = 17.146$ (@ 333 K) <sup>[8]</sup> , $10.97$ <sup>[58]</sup> Data from ref. <sup>[50]</sup> <table border="1"> <thead> <tr> <th colspan="3">50% point energy (J)</th> </tr> <tr> <th>3-mil foil</th> <th>10-mil foil</th> <th>% expl.</th> </tr> </thead> <tbody> <tr> <td>1.48</td> <td>10.79</td> <td>0</td> </tr> </tbody> </table>	50% point energy (J)			3-mil foil	10-mil foil	% expl.	1.48	10.79	0																																			
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$\Omega(\text{CO}_2)$ [%]	-55.9																																												

$T_{\text{m.p.}}$ [°C]	286–301 (dec.) <sup>[2]</sup> , 286 <sup>[3,4,12,17,18,32,47,48]</sup> , 282.1 (sample in sealed cell, DSC) <sup>[8]</sup> , 285 (DTA @ 10 °C/min) <sup>[7]</sup> , 287 <sup>[18]</sup> , 290 <sup>[18,32]</sup> , 280–288 <sup>[11]</sup> , 285 <sup>[28,39]</sup> , 287 (Thomas Hoover capillary melting point apparatus @ 2 °C/min) <sup>[32]</sup> , 288–290 (crude product) <sup>[42]</sup> , 280 (yellow needles) <sup>[42]</sup>																	
$T_{\text{subl.}}$ [°C]	200 mg sample rapidly disappears either subliming (or boiling) @ 335 °C completely in 5 s without apparent dec. <sup>[12]</sup> , rapid sublimation without apparent dec. when small quantities suddenly exposed to $T \gg$ deflgration point of 2 lb slab <sup>[12]</sup>																	
$T_{\text{phase transition}}$ [°C]	Form I is stable <217 °C <sup>[2,3]</sup> , 217 (form I–form II) <sup>[3]</sup> , ~220 (form I–form II) <sup>[7]</sup> , 216 (transformation to crystal form of lower $\rho$ ) <sup>[47]</sup> , two cryst. forms: low $T$ form I transforms to high $T$ form II >217 °C (microscopic observation and X-ray powder diffraction) <sup>[48]</sup> , form II persists for prolonged periods of time < transition temperature <sup>[48]</sup> , form II heated at 190, 200 and 210 °C showed no transformation after 7 h at these temperatures <sup>[48]</sup> , form II–form I solid–solid transition improbable under practical conditions <sup>[48]</sup> , rapid form II–form I transition under $\gamma$ -butyrolactone @ RT (transition completed within 4–6 h) <sup>[48]</sup> , form II–form I transition under acetone or dioxane @ RT also possible but required longer than under $\gamma$ -butyrolactone (transition completed within 4–6 h) <sup>[48]</sup> , melt solidifies to form II <sup>[48]</sup> , rapid cooling of a conc. DATB/ $\gamma$ -butyrolactone soln. near its bpt. forms a mixture of forms I and II <sup>[48]</sup>																	
$T_{\text{dec.}}$ [°C]	301 <sup>[11]</sup> , 360 (exotherm peak max., DSC @ 20 °C/min) <sup>[17]</sup> , 329.9 (extrapolated dec., onset $T$ , sample in sealed cell, DSC) <sup>[8]</sup> , 609.7 K (DSC) <sup>[53]</sup>																	
$\rho$ [g cm <sup>-3</sup> ]	1.837 (polymorph I, max. $\rho$ ) <sup>[2]</sup> , 1.815 (polymorph II) <sup>[2]</sup> , 1.79 (nominal) <sup>[2]</sup> , 1.837 <sup>[3]</sup> , 1.837 (@ TMD) <sup>[7,12]</sup> , 1.70 (nominal) <sup>[7]</sup> , 1.84 <sup>[24,49,55]</sup> , 1.84 (TMD) <sup>[8]</sup> , 1.76 (pressed, 96% TMD @ 64,000 psi loading pressure) <sup>[12]</sup> , 1.800 (exptl. $\rho$ , 98.2% TMD) <sup>[12,26]</sup> , 1.837 (crystal) <sup>[26]</sup> , 1.65 (@ 50,000 psi) <sup>[42]</sup> , 1.837 <sup>[47]</sup> , 1.837 (crystal, flotation method @ 23 °C, DATB I) <sup>[48]</sup> , 1.815 (crystal, flotation method @ 23 °C, DATB II) <sup>[48]</sup>																	
Data from ref. <sup>[3]</sup>																		
<table border="1"> <thead> <tr> <th rowspan="2">Method of determination</th> <th rowspan="2">State</th> <th rowspan="2"><math>T</math> (°C)</th> <th colspan="2">Density (g/cm<sup>3</sup>)</th> </tr> <tr> <th>Form I</th> <th>Form II</th> </tr> </thead> <tbody> <tr> <td>X-ray</td> <td>Solid</td> <td>23</td> <td>1.838</td> <td>1.84</td> </tr> <tr> <td>Direct measurement</td> <td>Solid</td> <td>23</td> <td>1.837</td> <td>1.815</td> </tr> </tbody> </table>		Method of determination	State	$T$ (°C)	Density (g/cm <sup>3</sup> )		Form I	Form II	X-ray	Solid	23	1.838	1.84	Direct measurement	Solid	23	1.837	1.815
Method of determination	State				$T$ (°C)	Density (g/cm <sup>3</sup> )												
		Form I	Form II															
X-ray	Solid	23	1.838	1.84														
Direct measurement	Solid	23	1.837	1.815														
DATB powder can be pressed into pellets <sup>[3]</sup>																		
Heat of formation	−23.6 kcal/mol ( $\Delta H_f^\circ$ ) <sup>[2,3]</sup> , −122 kJ/mol <sup>[7]</sup> , −98.8 kJ mol <sup>-1</sup> ( $\Delta H_f$ ) <sup>[24]</sup> , −97.1 kcal/kg ( $\Delta H_f$ ) <sup>[8]</sup> , −97.1 to −119 cal/g <sup>[2]</sup> , −503 kJ/kg <sup>[7]</sup> , −29.23 kcal/g <sup>[7]</sup> , −29.23 kcal mol <sup>-1</sup> <sup>[12]</sup> , −29.23 kcal/mol <sup>[26]</sup> , −120.0 kcal/kg (enthalpy of formation) <sup>[31]</sup> , −98.7 kJ/mol ( $\Delta H_f$ ) <sup>[49]</sup> , −97.9 kJ/mol (enthalpy of form., exptl.) <sup>[51]</sup> , −90.2 kJ/mol (enthalpy of form., calcd., emp.) <sup>[51]</sup> , −110.3 kJ/mol (enthalpy of form., calcd., S-D method) <sup>[51]</sup>																	
Heat of combustion	−7115 kcal/mol <sup>[2]</sup> , $\Delta H^\circ_c = -711.5 \text{ kcal/mol}$ <sup>[3]</sup>																	

	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^{\circ} \text{ [kJ kg}^{-1}\text{]}$		126 kcal/g [H <sub>2</sub> O (l)] (calcd. using rxn. enthalpies) <sup>[2,7]</sup>  115 kcal/g [H <sub>2</sub> O (g)] (calcd. using rxn. enthalpies) <sup>[2,7]</sup>  2,860 (@ 1.80 g cm <sup>-3</sup> , calcd. BKWR) <sup>[1]</sup>  2,870 (@ 1.78 g cm <sup>-3</sup> , calcd. BKWR) <sup>[1]</sup>  3,550 (@ 1.80 g cm <sup>-3</sup> , calcd. BKWS) <sup>[1]</sup>  3,550 (@ 1.78 g cm <sup>-3</sup> , calcd. BKWS) <sup>[1]</sup>  1,048 cal/g <sup>[20]</sup>  875 cal/g (@ 1.6 g cm <sup>-3</sup> , Q, calcd. Halford– Kistiakowsky equation of state) <sup>[26]</sup>  915 kcal/kg (@ 1.500 g cm <sup>-3</sup> , calcd.) [H <sub>2</sub> O vapor] <sup>[31]</sup>  $-\Delta H_{\text{det}} = 4.91 \text{ kJ/g}$ <sup>[49]</sup>	980 cal/g [H <sub>2</sub> O (l)] <sup>[2,7]</sup>  910 cal/g [H <sub>2</sub> O (g)] <sup>[2,7]</sup>  0.98 kcal/g [H <sub>2</sub> O (l)] <sup>[14]</sup>  800 cal/g (det. energy) <sup>[12,26]</sup>  930 kcal/kg (@ 1.500 g cm <sup>-3</sup> ) [H <sub>2</sub> O vapor] <sup>[31]</sup>  2,876 cal/g <sup>[42]</sup>
$T_{\text{ex}} \text{ [K]}$		2,638 (@ 1.6 g cm <sup>-3</sup> , calcd. Halford– Kistiakowsky equation of state) <sup>[26]</sup>	
$p_{\text{C-J}} \text{ [kbar]}$		250 (calcd., Ruby code) <sup>[7]</sup>  292 (@ 1.80 g cm <sup>-3</sup> , calcd. BKWR) <sup>[1]</sup>	251 <sup>[1,3,12,26]</sup>  259 (@ 1.78 g cm <sup>-3</sup> ) <sup>[2,7]</sup>

		<p>280 (@ 1.78 g cm<sup>-3</sup>, calcd. BKWR)<sup>[1]</sup></p> <p>258 (@ 1.80 g cm<sup>-3</sup>, calcd. BKWS)<sup>[1]</sup></p> <p>250 (@ 1.78 g cm<sup>-3</sup>, calcd. BKWS)<sup>[1]</sup></p> <p>261 (@ 1.788 g cm<sup>-3</sup>, calcd., empirical, <i>Xiong</i>)<sup>[20]</sup></p> <p>267 (calcd. K-J)<sup>[10]</sup></p> <p>170.3 (@ 1.6 g cm<sup>-3</sup>, calcd. Halford– Kistiakowsky equation of state)<sup>[26]</sup></p> <p>251 (@ 1.780 g cm<sup>-3</sup>)<sup>[2]</sup></p> <p>259 (@ 1.790 g cm<sup>-3</sup>)<sup>[2]</sup></p> <p>262 (@ 1.77 g cm<sup>-3</sup>, calcd.)<sup>[55]</sup></p>	<p>259 (@ 1.788 g cm<sup>-3</sup>)<sup>[20]</sup></p> <p>259<sup>[14]</sup></p>
VoD [m s <sup>-1</sup> ]		<p>7,920 (@ 1.80 g cm<sup>-3</sup>, calcd. BKWR)<sup>[1]</sup></p> <p>7,850 (@ 1.78 g cm<sup>-3</sup>, calcd. BKWR)<sup>[1]</sup></p> <p>7,860 (@ 1.80 g cm<sup>-3</sup>, calcd. BKWS)<sup>[1]</sup></p> <p>7,790 (@ 1.78 g cm<sup>-3</sup>, calcd. BKWS)<sup>[1]</sup></p> <p>7,690 (@ 1.84 g cm<sup>-3</sup> (TMD), calcd. empirical, R-P method)<sup>[15]</sup></p> <p>8,150 (@ 1.84 g cm<sup>-3</sup> (TMD), calcd. Aizenshtadt method)<sup>[15]</sup></p> <p>7,630 (@ 1.84 g cm<sup>-3</sup> (TMD), calcd. K-J)<sup>[15]</sup></p>	<p>7,600 (@ 1.80 g cm<sup>-3</sup>)<sup>[1,12,26]</sup></p> <p>7,585 (@ 1.79 g cm<sup>-3</sup>)<sup>[2]</sup></p> <p>7,600 (@ 1.78 g cm<sup>-3</sup>)<sup>[1,3,14]</sup></p> <p>7,500 (@ 1.788 g cm<sup>-3</sup>)<sup>[20]</sup></p> <p>6,330 (@ 1.49 g cm<sup>-3</sup>)<sup>[14]</sup></p> <p>7,500 (@ 1.65 g cm<sup>-3</sup>)<sup>[11]</sup></p> <p>7,690 (@ 1.837 g cm<sup>-3</sup>)<sup>[10]</sup></p> <p>7,520 (@ 1.79 cm<sup>-3</sup>)<sup>[7]</sup></p>

		7,684 (@ 1.788 g cm <sup>-3</sup> , calcd., empirical, <i>Xiong</i> ) <sup>[20]</sup>  7,520 (@ 1.79 g cm <sup>-3</sup> ) <sup>[20]</sup>  7,520 (@ 1.84 g cm <sup>-3</sup> , calcd. K-J) <sup>[7]</sup>  7,710 (@ 1.837 g cm <sup>-3</sup> , calcd. K-J) <sup>[10]</sup>  7,010 (@ 1.6 g cm <sup>-3</sup> , calcd. Halford– Kistiakowsky equation of state) <sup>[26]</sup>  7,690 (@ 1.77 g cm <sup>-3</sup> , calcd.) <sup>[55]</sup>										
$V_0$ [L kg <sup>-1</sup> ]		0.4865 cm <sup>3</sup> /g (@ 1.6 g cm <sup>-3</sup> , calcd. Halford–Kistiakowsky equation of state) <sup>[26]</sup>										
<hr/>												
Critical diameter [cm]	5.3 mm (unconfined, @ 1.816 g cm <sup>-3</sup> ) <sup>[2,3]</sup> , 5.3 mm (@ 1.78–1.80 g cm <sup>-3</sup> ) <sup>[19]</sup> critical heights and diameters <sup>[23]</sup> : pressed DATB: $\rho_0 = 1.724$ g cm <sup>-3</sup> ; wedge height, $h_c = 0.73$ mm, $d_c = 5.3$ mm, $d_c$ (lit. value) = 25, $d_c / h_c = 7.3$ <sup>[23]</sup> , $d_c = 5.3$ mm ( $\rho = 1.800$ g cm <sup>-3</sup> , 97.9% TMD) <sup>[23,25]</sup> , fine DATB, critical diameter for detonation $d_c = 5.3$ mm <sup>[41]</sup> , pressed DATB, $\rho = 1.800$ g/cc, 97.9% TMD, $d_c = 0.53$ cm <sup>[46]</sup> ; 50% point $\rho_0 = 1.80$ g/cc, 97.9% TMD, $P_g = 53$ kbar by extrapolation <sup>[46]</sup>											
Critical $T$ [°C]	320–323 (exptl.) <sup>[34,38]</sup> , 323 (calcd.) <sup>[34,38]</sup> , 322 <sup>[3]</sup>											
Sand test [g]	120% TNT <sup>[2]</sup>											
Underwater small-scale gap test	Critical length, $L_c = 3$ mm <sup>[8]</sup>											
Gap test	PX gap test values <sup>[2]</sup> :  <table border="1"> <thead> <tr> <th>Density (g/cm<sup>3</sup>)</th> <th>% voids</th> <th>Sensitivity (mm)</th> </tr> </thead> <tbody> <tr> <td>1.781</td> <td>3.2</td> <td>17.86</td> </tr> <tr> <td>1.446</td> <td>21.3</td> <td>19.94</td> </tr> </tbody> </table>			Density (g/cm <sup>3</sup> )	% voids	Sensitivity (mm)	1.781	3.2	17.86	1.446	21.3	19.94
Density (g/cm <sup>3</sup> )	% voids	Sensitivity (mm)										
1.781	3.2	17.86										
1.446	21.3	19.94										

LSGT [cm]	LANL large-scale gap test <sup>[2]</sup> :					
	Density (g/cm <sup>3</sup> )	% voids	Sensitivity (mm)			
$G_{50} = 49.27 \text{ mm}$ , $L_{95} = 0.23 \text{ mm}$ (@ 0.81 g cm <sup>-3</sup> ) <sup>[3]</sup> , $G_{50} = 45.36 \text{ mm}$ , $L_{95} = 0.08 \text{ mm}$ (@ 1.705 g cm <sup>-3</sup> ) <sup>[3]</sup> , $G_{50} = 41.68 \text{ mm}$ , $L_{95} = 0.18 \text{ mm}$ (@ 1.786 g cm <sup>-3</sup> ) <sup>[3]</sup> , $G_{50} = 41.7 \text{ mm}$ (@ 1.77 g cm <sup>-3</sup> , pressed) <sup>[3]</sup> , 41.68 mm (LASL, LSGT) <sup>[19]</sup> , 27 mm (NOL) <sup>[27]</sup> , 42 mm (LANL) <sup>[27]</sup> , $L_g = 136 \text{ in} \times 10^2$ (@ 1.80 g cm <sup>-3</sup> , 97.9% TMD, NSWC LSGT) <sup>[23]</sup> , $L_g = 179 \text{ in} \times 10^2$ (@ 1.705 g cm <sup>-3</sup> , 92.8% TMD, hot-pressed, LASL LSGT) <sup>[23]</sup> , $L_g = 164 \text{ in.} \times 10^2$ (@ 1.786 g cm <sup>-3</sup> , 97.2% TMD, hot-pressed, LASL LSGT) <sup>[23]</sup> , $L_g = 132 \text{ in} \times 10^2$ (@ 1.70 g cm <sup>-3</sup> , 92.5% TMD, hot-pressed, LASL NSWC) <sup>[23]</sup>						
Conversion of SSGT values to LSGT values <sup>[41]</sup> :						
$\rho_0$ (g/cc)	% TMD	50% point				
		DBG	SSGT, $P_g$ (kbar)	LSGT, $P_g$ (kbar)		
	1.233	67.12	6.94	31.2	25.0	
	1.455	79.20	7.38	35.8	28.5	
	1.601	87.15	7.88	42.2	33.2	
	1.676	91.24	8.10	45.3	34.8	
	1.761	95.86	9.00	60.8	43.2	
$\rho_0 = 1.21 \text{ g/cc}$ , 65.8% TMD, 50% pressure ( $P_g$ ) = 31.1 kbar <sup>[46]</sup>						
Data from ref. <sup>[46]</sup> :						
Density (g/cc)	% TMD	50% point			Particle size (μm)	Comments
		Cards	kbar			
	1.211	65.8	162	31	8	From Holston ordnance
	1.441	78.1	151	36	8	
	1.701	92.5	132	45	8	
	1.711	92.9	135	(44)		Ball-milled, from Picatinny
	1.671	90.7	139	44	11	0.37 g/cc bulk density
	1.671	90.9	140	44	11	
	1.671	91.0	139	44	11	
	1.671	91.1	138	(42)	11	

SSGT [cm]	Values from ref. <sup>[2]</sup>			
	Test type	Density (g/cm <sup>3</sup> )	% voids	Sensitivity (mm)
NSWC SSGT	1.775	3.5	3.28	
	1.233	33	5.18	
LANL SSGT	1.801 (hot pressed)	2.0	0.36	
	1.714 (pressed)	6.7	1.27	
$G_{50} = 0.36 \text{ mm}$ , $L_{95} = 0.10 \text{ mm}$ (@ 1.801 g cm <sup>-3</sup> ) <sup>[3]</sup> , 3.0 mm (NOL) <sup>[27]</sup> , 0.3 mm (LANL) <sup>[27]</sup>				
Small-scale gap (booster) sensitivity test <sup>[12]</sup> :				
Pressed composition	@ 93% TMD		@ 95% TMD	
	DBG	Lucite gap (mils)	DBG	Lucite gap (mils)
	DATB	8.4 145	8.8	132
DBG = 30–101 g (test gap/ref. gap)				
Sensitivity change with density <sup>[12]</sup> :				
Loading pressure (psi)	$\rho$ (g cm <sup>-3</sup> )	% TMD	DBG	Lucite gap (in mils)
	1.233	67.1	6.938	202
	1.455	79.2	7.375	183
	1.601	87.2	7.875	163
	1.676	91.2	8.100	155
	1.763	96.0	9.000	126
Conversion of SSGT values to LSGT values <sup>[41]</sup> :				
$\rho_0$ (g/cc)	% TMD	50% point		
		DBG	SSGT, $P_g$ (kbar)	LSGT, $P_g$ (kbar)
1.233	67.12	6.94	31.2	25.0
1.455	79.20	7.38	35.8	28.5
1.601	87.15	7.88	42.2	33.2
1.676	91.24	8.10	45.3	34.8
1.761	95.86	9.00	60.8	43.2

TMD = 1.84, data from ref.<sup>[45]</sup>:

Loading pressure (kpsi)	Density (g/cm <sup>3</sup> )		% TMD	Sensitivity (DBG.)			
	AVG	s		AVG.	g	s <sub>m</sub>	N
50.2	1.732	0.0072	94.1	8.535	0.0329	0.0137	46

TMD = 1.84, (1) = no mixed response zone, data from ref.<sup>[45]</sup>:

Loading pressure (kpsi)	Density (g/cm <sup>3</sup> )		% TMD	Sensitivity (DBG.)			
	AVG	s		AVG.	g	s <sub>m</sub>	N
4	1.233	0.0219	67.0	6.909	—	—	12 (1)
10	1.455	0.0087	79.1	7.411	—	—	8 (1)
32	1.676	0.0060	91.1	8.153	—	—	8 (1)
64	1.765	0.0057	95.8	9.006	0.837	0.0793	12

TMD = 1.84, data from ref.<sup>[45]</sup>

Loading pressure (kpsi)	Density (g/cm <sup>3</sup> )		% TMD	Sensitivity (DBG.)			
	AVG	s		AVG.	g	s <sub>m</sub>	N
4	1.255	0.0025	68.2	6.870	0.0103	0.0060	22
8	1.365	0.0043	74.2	7.042	0.0134	0.0196	20
16	1.518	0.0054	82.5	7.374	0.0122	0.0100	20
32	1.665	0.0034	90.5	8.023	0.0535	0.0316	20
64	1.775	0.0083	96.5	8.882	0.0443	0.0276	20

TMD = 1.84 g/cm<sup>3</sup>, steel dent output data from ref.<sup>[45]</sup>

Loading pressure (psi)	Density (g/cm <sup>3</sup> )		Group 1 data				Block hardness data (Rockwell 8)	
			Observed dent data (mils)		Corrected dent data (mils)			
	AVG.	s	AVG.	s	AVG.	s	AVG.	s
4,000	1.257	0.0066	41.4	1.57	42.6	1.49	84.8	1.60
8,000	1.384	0.0028	40.3	3.51	42.2	3.44	85.7	1.55
16,000	1.530	0.0047	49.2	2.54	49.4	3.84	83.3	1.99
32,000	1.663	0.0024	50.9	4.91	52.5	6.43	85.4	2.88
64,000	1.771	0.0041	53.2	2.20	53.7	2.31	83.7	1.72



	<p>@ 200 °C (total cm<sup>3</sup> gas evolved/no. days)<sup>[9]</sup>: 2.8/2, 3.6/7, 4.5/14, 5.5/21, 6.2/28, 7.4/35, 8.4/42, 9.5/49, 10.7/56, 11.8/63, 13.2/70, 14.7/77, 16.4/84<sup>[9]</sup></p> <p>@ 175 °C (total cm<sup>3</sup> gas evolved/no. days)<sup>[9]</sup>: 1.4/2, 1.8/7, 2.1/14, 2.3/21, 2.5/28, 2.7/35, 2.8/42, 2.9/49, 3.0/56, 3.2/63, 3.4/70, 3.6/77, 3.7/84, 3.8/91<sup>[9]</sup></p> <p>@ 150 °C (total cm<sup>3</sup> gas evolved/no. days)<sup>[9]</sup>: 0.6/2, 1.1/7, 1.5/14, 1.7/21, 1.7/28, 1.7/35, 1.8/42, 1.8/49, 1.9/56, 1.9/63, 2.0/70, 2.0/77, 2.0/84, 2.1/91<sup>[9]</sup></p>																																													
Thermal stability	<p>Dec. of ~ 10%/h @ 280 °C<sup>[39]</sup>, dec. rate &lt; 1%/h @ 260 °C<sup>[47]</sup>, dec. rate of 1–1.5% per h @ 260 °C<sup>[10]</sup>, 4–6 cc gas/g DATB/h<sup>[48]</sup>, 420 cc gas from 1 g DATB @ 260 °C (calcd.)<sup>[48]</sup>, 1–1.5% dec./h @ 260 °C<sup>[48]</sup>, approx. constant rate of dec. @ 260 °C for 6 h<sup>[48]</sup>, autocatalytic dec. @ 280 °C<sup>[48]</sup></p> <p>Dec. of DATB @ 280 °C, approx. values from graph<sup>[48]</sup>:</p> <table border="1"> <thead> <tr> <th>Time (min)</th> <th>% dec.</th> <th>Time (min)</th> <th>% dec.</th> </tr> </thead> <tbody> <tr> <td>20</td> <td>1.5</td> <td>80</td> <td>4.5</td> </tr> <tr> <td>40</td> <td>2</td> <td>100</td> <td>16</td> </tr> <tr> <td>60</td> <td>3</td> <td>120</td> <td>30</td> </tr> </tbody> </table>	Time (min)	% dec.	Time (min)	% dec.	20	1.5	80	4.5	40	2	100	16	60	3	120	30																													
Time (min)	% dec.	Time (min)	% dec.																																											
20	1.5	80	4.5																																											
40	2	100	16																																											
60	3	120	30																																											
Thermal conductivity	$6.19 \times 10^{-4}$ cal/s/cm/°C <sup>[3]</sup> , 0.261 × 10 <sup>-4</sup> cal/s/cm/°C <sup>[26]</sup>																																													
Specific heat [cal/g/°C]	$65.8^{[26]}$ , heat capacity = $0.20 + (1.11 \times 10^{-3})T - (1.81 \times 10^{-6})T^2$ (density = 1.834 g cm <sup>-3</sup> ) <sup>[3]</sup>																																													
Vapor pressure [atm @ °C]	<p><math>1.78 \times 10^{-8}</math> Torr (@ 6 °C)<sup>[5]</sup>, 0.081 mm Hg × 10<sup>7</sup> (@ 62.6 °C)<sup>[3]</sup>, 0.879 mm Hg × 10<sup>7</sup> (@ 78.2 °C)<sup>[3]</sup>, 2.09–2.36 mm Hg × 10<sup>7</sup> (@ 85.3 °C)<sup>[3]</sup>, 9.12–9.80 mm Hg × 10<sup>7</sup> (@ 97.6 °C)<sup>[3]</sup>, 34 mm Hg × 10<sup>7</sup> (@ 108.1 °C)<sup>[3]</sup></p> <p>Values from<sup>[40]</sup></p> <table border="1"> <thead> <tr> <th>T (°C)</th> <th>Vapor pressure (<math>\times 10^7</math> Torr)</th> <th>Wt. loss (g × 10<sup>3</sup>)</th> <th>Time (s)</th> <th>area (cm<sup>2</sup>)</th> </tr> </thead> <tbody> <tr> <td>62.6</td> <td>0.081</td> <td>3.3</td> <td>303,200</td> <td>6.33</td> </tr> <tr> <td>78.2</td> <td>0.879</td> <td>12.4</td> <td>459,360</td> <td>6.33</td> </tr> <tr> <td>85.3</td> <td>2.36</td> <td>4.9</td> <td>68,400</td> <td>6.33</td> </tr> <tr> <td>85.3</td> <td>2.25</td> <td>5.9</td> <td>86,400</td> <td>6.33</td> </tr> <tr> <td>85.3</td> <td>2.09</td> <td>5.1</td> <td>80,280</td> <td>6.33</td> </tr> <tr> <td>97.6</td> <td>9.80</td> <td>15.3</td> <td>52,200</td> <td>6.33</td> </tr> <tr> <td>97.6</td> <td>9.12</td> <td>15.9</td> <td>58,320</td> <td>6.33</td> </tr> <tr> <td>108.1</td> <td>34.0</td> <td>31.0</td> <td>30,960</td> <td>6.33</td> </tr> </tbody> </table> <p>Sublimes readily @ atmospheric pressure @ 200 °C<sup>[48]</sup></p>	T (°C)	Vapor pressure ( $\times 10^7$ Torr)	Wt. loss (g × 10 <sup>3</sup> )	Time (s)	area (cm <sup>2</sup> )	62.6	0.081	3.3	303,200	6.33	78.2	0.879	12.4	459,360	6.33	85.3	2.36	4.9	68,400	6.33	85.3	2.25	5.9	86,400	6.33	85.3	2.09	5.1	80,280	6.33	97.6	9.80	15.3	52,200	6.33	97.6	9.12	15.9	58,320	6.33	108.1	34.0	31.0	30,960	6.33
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Solubility [g/mL]	<p>Slightly soluble in acetic acid and only very slightly soluble in other solvents<sup>[2]</sup>, slightly soluble in hot glacial acetic acid, dioxane and nitrobenzene<sup>[39]</sup>, rather insoluble in MeOH, acetone, benzene and hexane<sup>[48]</sup>, slightly soluble in hot dioxane, nitrobenzene and glacial acetic acid<sup>[48]</sup>, rel. soluble in hot <math>\gamma</math>-butyrolactone<sup>[48]</sup>, 5 g/100 mL <math>\gamma</math>-butyrolactone @ 100 °C<sup>[48]</sup>, 10 g/100 mL <math>\gamma</math>-butyrolactone @ 125 °C<sup>[48]</sup>, 25 g/100 mL <math>\gamma</math>-butyrolactone @ 150 °C<sup>[48]</sup>, recryst. from DMF or DMSO<sup>[3]</sup>, insoluble in MeOH<sup>[3]</sup></p> <p>Solubility of DATB (g/100 g of solvent) after 5 min stirring; <sup>a</sup> at the boiling point of the solvent<sup>[44]</sup>:</p> <table border="1"> <thead> <tr> <th>Solvent</th><th>25 °C</th><th>60 °C</th><th>80 °C</th><th>98 °C</th></tr> </thead> <tbody> <tr> <td>DMSO</td><td>2.2</td><td></td><td></td><td>19</td></tr> <tr> <td>DMF</td><td>2.5</td><td>5.1</td><td>9.7</td><td>14</td></tr> <tr> <td><i>N</i>-Methylpyrrolidone</td><td>4.5</td><td></td><td></td><td>17</td></tr> <tr> <td>Butyrolactone</td><td>0.8</td><td></td><td></td><td>4.8</td></tr> <tr> <td>Acetone</td><td>0.4</td><td>1.4<sup>a</sup></td><td></td><td></td></tr> <tr> <td>Aniline</td><td>2.2</td><td></td><td></td><td></td></tr> <tr> <td>Trifluoroacetic acid</td><td>&lt;0.1</td><td></td><td></td><td></td></tr> </tbody> </table> <p>Solubility of DATB in binary solvent mixtures at 25 °C (g/100 g of solvent after 5 min stirring)<sup>[44]</sup>:</p> <table border="1"> <thead> <tr> <th>Solvent</th><th>g DATB/100 g solvent</th></tr> </thead> <tbody> <tr> <td>DMSO</td><td>2.2</td></tr> <tr> <td>NMP</td><td>4.5</td></tr> <tr> <td>NMP 79.2%</td><td>4.6</td></tr> <tr> <td>DMSO 20.8%</td><td></td></tr> <tr> <td>DMF</td><td>2.5</td></tr> <tr> <td>DMF 71.7%</td><td>2.9</td></tr> <tr> <td>DMSO 28.3%</td><td></td></tr> <tr> <td>Butyrolactone</td><td>0.8</td></tr> </tbody> </table> <p>Comparison of solubility (g/100 g DMSO solvent) after 5 and 30 min stirring at 25 °C: 2.2 g after 5 min<sup>[44]</sup>, 2.3 g after 30 min<sup>[44]</sup></p>	Solvent	25 °C	60 °C	80 °C	98 °C	DMSO	2.2			19	DMF	2.5	5.1	9.7	14	<i>N</i> -Methylpyrrolidone	4.5			17	Butyrolactone	0.8			4.8	Acetone	0.4	1.4 <sup>a</sup>			Aniline	2.2				Trifluoroacetic acid	<0.1				Solvent	g DATB/100 g solvent	DMSO	2.2	NMP	4.5	NMP 79.2%	4.6	DMSO 20.8%		DMF	2.5	DMF 71.7%	2.9	DMSO 28.3%		Butyrolactone	0.8
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	g DATB/100 g solvent @ 40 and 60 °C <sup>[3]</sup> :		
Solvent	40 °C	60 °C	
Acetic anhydride	0.492		
γ-Butyrolactone	0.810		
Cyclohexanone	0.355		
DMF	2.96	4.88	
DMSO	4.56	8.15	
Formamide	0.282		
Nitromethane	0.362		
Sulfuric acid	22.2	22.9	
Dipole moment [D]	1.48 (calcd.) <sup>[17]</sup>		
Wedge test [mm]	0.57 (LANL) <sup>[27]</sup>		
Min prim charge test [mg]	Minimum priming charge <sup>[3]</sup> :		
	Density (g/cm <sup>3</sup> )	$W_{50}$ (mg of XTX 8003)	$L_{95}$ ( $\pm \log$ mg)
	1.783	57.1	0.108
	56 (LANL) <sup>[27]</sup> , $\rho = 1.707$ g cm <sup>-3</sup> , $W_{50} = 26$ mg (minimum priming weight) <sup>[3]</sup>		
Detonation failure thickness	Data from ref. <sup>[3]</sup>		
	Density (g/cm <sup>3</sup> )	Failure thickness (mm)	$L_{95}$ (mm)
	1.708	0.630	0.069
	1.724	0.732	0.145
$\Delta H_{\text{sub}}$ [kJ/mol]	Heat of subl. = 138 cal/g <sup>[2]</sup> , 143.5 (exptl.) <sup>[35]</sup> , 154.8 (calcd., QSPR) <sup>[35]</sup> , 33.47 kcal (molar heat of sublimation) <sup>[40]</sup> , 137.6 cal/g (specific heat of sublimation) <sup>[40]</sup> , 33.47 kcal/mol (latent heat, solid form I to gas, calcd. from vapor pressure data) <sup>[3]</sup>		
Cook-off test	8 min @ 320 °C <sup>[42]</sup>		
Plate dent test	Brisance = 120% TNT <sup>[2]</sup>		
$Q_{\text{dec.}}$ [kJ/mol]	1,097 (DSC) <sup>[53]</sup>		

Radiation sensitivity	Data from ref. <sup>[56]</sup>																									
	Exposure rate (R/h)	Total dose (R)	Vacuum stability test																							
			100 °C (cc/g/40 h)	120 °C (cc/g/40 h)	200 °C (cc/2 g/2 h)																					
	$9.2 \times 10^5$	Control			0.20																					
		$1.5 \times 10^7$			0.28																					
		$1.3 \times 10^8$			0.42																					
		$1.2 \times 10^9$			0.90																					
		$4.0 \times 10^9$			6.15 (marginal)																					
Dimensional changes in explosive pellets as function of total gamma exposure <sup>[56]</sup> :																										
<table border="1"> <thead> <tr> <th>Total exposure (R)</th><th>Weight loss (%)</th><th>Diameter change (%)</th><th>Length change (%)</th><th>density change (%)</th></tr> </thead> <tbody> <tr> <td><math>1.1 \times 10^7</math></td><td>0.02</td><td>n.c.</td><td>n.c.</td><td>n.c.</td></tr> <tr> <td><math>1.3 \times 10^8</math></td><td>0.1</td><td>n.c.</td><td>+ 0.13</td><td>- 0.4</td></tr> <tr> <td><math>1.1 \times 10^9</math></td><td>0.3</td><td>n.c.</td><td>+ 0.13</td><td>- 0.5</td></tr> </tbody> </table>							Total exposure (R)	Weight loss (%)	Diameter change (%)	Length change (%)	density change (%)	$1.1 \times 10^7$	0.02	n.c.	n.c.	n.c.	$1.3 \times 10^8$	0.1	n.c.	+ 0.13	- 0.4	$1.1 \times 10^9$	0.3	n.c.	+ 0.13	- 0.5
Total exposure (R)	Weight loss (%)	Diameter change (%)	Length change (%)	density change (%)																						
$1.1 \times 10^7$	0.02	n.c.	n.c.	n.c.																						
$1.3 \times 10^8$	0.1	n.c.	+ 0.13	- 0.4																						
$1.1 \times 10^9$	0.3	n.c.	+ 0.13	- 0.5																						
DTA for irradiated DATB @ 20 °C/min <sup>[56]</sup> :																										
	Total dose (R)	Endotherms				exotherms																				
		First		Second		First																				
		Onset (°C)	Peak (°C)	Onset (°C)	Peak (°C)	Onset (°C)	Peak (°C)																			
	0	223	227	265	282	295	313																			
	$1.5 \times 10^7$	213	220	260	281	290	318																			
	$1.3 \times 10^8$	215	224	255	280	295	334																			
	$1.2 \times 10^9$	230	236	264	276	290	349																			
	$4.0 \times 10^9$	233	240	250	273	300	343																			
TGA for irradiated DATB <sup>[56]</sup> :																										
	Total dose (R)	Heating rate (°C/min)	Weight (mg)	Start of dec (°C)	10% weight loss T (°C)	Total weight loss (%)	Remarks																			
		20	7.9	215	275	96 @ 345 °C	-																			
		$1.5 \times 10^7$	8.6	215	275	96 @ 335 °C	-																			
		$1.3 \times 10^8$	7.9	215	275	96 @ 350 °C	-																			
		$1.2 \times 10^9$	8.1	215	283	92 @ 350 °C	-																			

Total dose (R)	Heating rate (°C/min)	Weight (mg)	Start of dec (°C)	10% weight loss T (°C)	Total weight loss (%)	Remarks
$4.0 \times 10^9$	20	7.65	180	272	82 @ 340 °C	-
0	10	9.8	200	254	97 @ 330 °C	-
$1.3 \times 10^8$	10	9.9	195	252	97 @ 310 °C	-
$1.2 \times 10^9$	10	9.4	195	268	93 @ 330 °C	-
0	50	8.4	215	281	93 @ 335 °C	-
$1.3 \times 10^8$	50	8.8	205	282	97 @ 360 °C	-
$1.2 \times 10^9$	50	8.2	255	300	-	Deflagrated @ 358 °C
0	80	10.2	230	326	97 @ 410 °C	-
$1.3 \times 10^8$	80	8.1	210	290	97 @ 355 °C	-
$1.2 \times 10^9$	80	9.3	220	315	92 @ 395 °C	Partial deflagration @ 373 °C

Effect of gamma radiation on the mpt. and color<sup>[56]</sup>:

Total dose (R)	Mpt. (°C)	Color
0	283.5	Yellow
$1.5 \times 10^7$	283.5	Yellow green
$1.3 \times 10^8$	282.5	Green
$1.2 \times 10^9$	281.5	Dark brown
$4.0 \times 10^9$		Purplish brown

IS for irradiated explosives, 50% fire height in inches, Bruceton method (P.A. apparatus, 2 kg mass)<sup>[56]</sup>:

Total Co <sup>60</sup> gamma dose (R)	Mean (in)	$\sigma$ std. dev. (in)
0	20.64	6.20
$1.5 \times 10^7$	19.00	1.26
$1.3 \times 10^8$	17.80	1.99
$1.2 \times 10^9$	13.50	1.51

Effect of gamma radiation on explosion T (5 s explosion T in °C) and activation energy (kcal/mol)<sup>[56]</sup>:

	Total dose (R)	5 s explosion T (°C)	Apparent activation energy (kcal/mol)
0	396	14.44	
$1.5 \times 10^7$	384	17.83	
$1.3 \times 10^8$	373	15.95	
$1.2 \times 10^9$	365	17.74	

Effect of gamma radiation on rates of detonation <sup>[56]</sup> :				
Total dose (R)	Density (g/cc)	Density after irradiation (g/cc)	Rate of detonation (m/s)	Detonation pressure (kbar)
0	1.80	—	7,600	260
0	1.49	—	6,630	164
$1.1 \times 10^7$	1.66	1.66	7,185	214
$1.3 \times 10^8$	1.66	1.65	7,180	213
$1.1 \times 10^9$	1.71	1.70	7,235	218

Plate push value @ 98% TMD = 3,130 ft/s<sup>[12,26]</sup>, plate push value @ 93% TMD = 3,028 ft/s (calcd. from values measured @ other ρ)<sup>[12,26]</sup>, failure diameter = 0.53 cm<sup>[12,26]</sup>

VoD exptl. determined values<sup>[26]</sup>:

Charge no.	Diameter (cm)	Length (cm)	Confinement	$\rho$ (g/cm <sup>3</sup> )	VoD (m/s)
1 <sup>†</sup>	Conical*	1.250	None	1.816	‡
	0.64	2.540	None	1.816	7,620
	1.27	2.644	None	1.815	7,620
	2.54	7.861	None	1.809	7,620
2	5.47	13.40	Glass	0.901	5,050
3	5.47	15.31	Lucite <sup>§</sup>	1.427	6,600
4	4.48	15.53	Lucite <sup>§</sup>	1.375	6,470
5	4.44	15.26	Al	1.381	6,470
6	4.44	15.27	Al	1.285	6,130
7	4.44	15.27	Al	1.205	5,880
8	5.08	15.80	None	1.788	7,570
9	5.08	20.47	None	1.793	7,580

<sup>†</sup>Charge 1 was in the form of a pyramid composed of cylinders, plus a conical apex;

<sup>\*</sup>failure diameter = 0.53 cm; <sup>‡</sup>diameter uniformly decreased from 0.64 to 0.32 cm over 1.25 cm length;

<sup>§</sup>wall thickness = 0.20 cm<sup>[26]</sup>

Chapman–Jouguet pressure, energy and isentropic exponent from H<sub>2</sub>O shock measurements<sup>[26]</sup>:

Explosive	$\rho$ (g/cm <sup>3</sup> )	VoD (m/s)	$U_{H_2O}$ (m/s)	$u_{H_2O}$ (m/s)	$P_{H_2O}$ @ HE.H <sub>2</sub> O interface (kb)	$P_{CJ}$ (kb)	$k$	$Q$ (cal/g)
DATB	1.79	7,585	5,980	2,624	156.9	251.0	3.10	800
DATB/Zytel (95:5)	1.71	7,200	5,839	2,524	147.4	224.0	2.97	797

Wedge test parameters<sup>[26]</sup>:

Brass thickness (cm)	Initial shock velocity H.E. (m/s)	Initial particle velocity H.E. (m/s)	Initial shock pressure H.E. (kb)	Initial compression H.E. ( $v/v_0$ )	$\rho_0$ H.E. (g/cm <sup>3</sup> )	D (final) (m/s)
1.27	4,670	1167	99.2	0.750	1.820	7,640
1.27	4,660	1167	99.3	0.750	1.825	7,460
2.54	4,870	972	85.4	0.800	1.803	7,620
2.54	4,700	979	82.8	0.792	1.799	7,700
3.81	4,736	892	76.6	0.810	1.813	7,590
3.81	4,767	892	76.5	0.815	1.810	7,500

	DATB <sup>[4]</sup>	DATB <sup>[13]</sup>	DATB form I <sup>[2,3,4]</sup> (stable from RT to 217 °C)	DATB form II <sup>[2,3,4]</sup> (stable from 217 to 286 °C)	DATB I <sup>[48]</sup>	DATB II <sup>[48]</sup>
Chemical formula	C <sub>6</sub> H <sub>5</sub> N <sub>5</sub> O <sub>6</sub>	C <sub>6</sub> H <sub>5</sub> N <sub>5</sub> O <sub>6</sub>	C <sub>6</sub> H <sub>5</sub> N <sub>5</sub> O <sub>6</sub>	C <sub>6</sub> H <sub>5</sub> N <sub>5</sub> O <sub>6</sub>	C <sub>6</sub> H <sub>5</sub> N <sub>5</sub> O <sub>6</sub>	C <sub>6</sub> H <sub>5</sub> N <sub>5</sub> O <sub>6</sub>
Molecular weight [g mol <sup>-1</sup> ]	243.14	243.14	243.14	243.14	243.14	243.14
Crystal system	Monoclinic	Monoclinic	Monoclinic		Monoclinic	Monoclinic
Space group	Pc (no. 7)	Pc (no. 7)	Pc (no. 7)		Pc	
$a$ [Å]	7.300(10)	7.309(3)	7.30 ± 0.01	7.76	7.26	7.76
$b$ [Å]	5.200(10)	5.169(4)	5.20 ± 0.01	9.04	5.21	9.04

$c$ [Å]	11.630(20)	11.583(2)	11.63 ± 0.02	12.84	11.68	12.84
$\alpha$ [°]	90	90	90	90	90	90
$\beta$ [°]	95.90(30)	95.22(2)	95.8 ± 0.3	103.0	96	103
$\gamma$ [°]	90	90	90	90	90	90
$V$ [Å <sup>3</sup> ]	439.136	435.8(4)	439.3		440	877
$Z$	2	2	2	4	2	4
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.839	1.853	1.838	1.84	1.835	1.84
$T$ [K]	295	223.2	RT			

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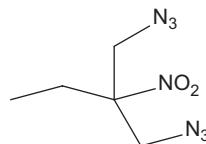
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## 1,3-Diazido-2-ethyl-2-nitropropane

Name [German, acronym]: Diazidoethylnitropropane, [1,3-diazido-2-ethyl-2-nitropropan, DAENP]

Main (potential) use: Potential new energetic plasticizer<sup>[1]</sup>

Structural formula:



	<b>DAENP</b>		
Formula	C <sub>5</sub> H <sub>9</sub> N <sub>7</sub> O <sub>2</sub>		
Molecular mass [g mol <sup>-1</sup> ]	199.17		
Appearance at RT			
IS [J]	$H_{50} > 170$ cm (2 kg mass) <sup>[1]</sup>		
FS [N]	>36 kg (Julius-Peters apparatus, 0/5 ignitions) <sup>[1]</sup>		
N [%]	49.23		
$\Omega(\text{CO}_2)$ [%]	-100.4		
T <sub>m.p.</sub> [°C]	-5.86 (DSC @ 10 °C/min, 1–2 mg sample, hermetically sealed Al cup, N <sub>2</sub> flow) <sup>[1]</sup>		
T <sub>crystallization</sub> [°C]	-25.80 (DSC @ 10 °C/min, 1–2 mg sample, hermetically sealed Al cup, N <sub>2</sub> flow) <sup>[1]</sup>		
T <sub>glass transition</sub> [°C]	-96.73 (DSC @ 10 °C/min, 1–2 mg sample, hermetically sealed Al cup, N <sub>2</sub> flow) <sup>[1]</sup>		
T <sub>dec.</sub> [°C]	219.6 (onset), 245.5 (peak max.) (DSC @ 10 °C/min, 1–2 mg sample, hermetically sealed Al cup, N <sub>2</sub> flow) <sup>[1]</sup> , 254 (TGA) <sup>[1]</sup>		
$\rho$ [g cm <sup>-3</sup> ]	1.32 <sup>[1]</sup>		
Heat of formation	464 kJ/mol ( $\Delta H_f$ , calcd.) <sup>[1]</sup>		
	Calcd. (EXPL05 6.04)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^\circ$ [kJ kg <sup>-1</sup> ]			
T <sub>ex</sub> [K]			
p <sub>C-J</sub> [kbar]			

VoD [ $\text{m s}^{-1}$ ]			
$V_0$ [ $\text{L kg}^{-1}$ ]			
Thermal stability	Stable <179 °C, single step dec. @ 254 °C with ~ 90% weight loss <389 °C <sup>[1]</sup>		
Compatibility	Compatible with GAP <sup>[1]</sup> , BAMP-THF copolymer <sup>[1]</sup> and polyNIMMO <sup>[1]</sup>		
Energy of dec. [J/g]	2056 <sup>[1]</sup>		
$\Delta H_{\text{melt}}$ [J/g]	47.8 <sup>[1]</sup>		

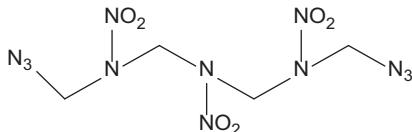
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## 1,7-Diazido-2,4,6-trinitro-2,4,6-triazaheptane

Name [German, acronym]: 1,7-Diazido-2,4,6-trinitro-2,4,6-triazaheptane,  
 [1,7-diazido-2,4,6-trinitro-2,4,6-triazaheptan, DATH]

Main (potential) use: plasticizer

Structural formula:



	DATH
Formula	C <sub>4</sub> H <sub>8</sub> N <sub>12</sub> O <sub>6</sub>
Molecular mass [g mol <sup>-1</sup> ]	320.19
Appearance at RT	Colorless polycrystalline solid <sup>[1]</sup> , soft waxy, transparent film (unstable amorphous state @ RT) which gradually transforms into opaque crystalline film after ~60 min <sup>[1]</sup> , amorphous phase, unstable @ RT, by rapid removal of solvent or rapid cooling of melt <sup>[2]</sup> , transparent waxy material which transforms into crystalline material over 60 min <sup>[2]</sup> , crystals obtained by slow evaporation of solvent <sup>[2]</sup>
N [%]	52.5
$\Omega(\text{CO}_2)$ [%]	-30.0
T <sub>m.p.</sub> [°C]	406 K (DTA, 1–2 mg sample, @ 5 K/min) <sup>[1]</sup>
T <sub>phase transition</sub> [°C]	Rapid evaporation of a DATH soln. or cooling molten DATH produces unstable amorphous phase but slow evaporation forms stable crystalline state <sup>[1]</sup> , amorphous state slowly crystallizes <335 K <sup>[1]</sup> , crystallization rate requires ~ 20 min @ 302 K but 150 min @ 287 K <sup>[1]</sup> , amorphous phase exists from mpt. -333 to 209 K range (DTA) <sup>[1]</sup> , crystalline DATH does not transform to amorphous phase on heating (DTA) <sup>[1]</sup> , amorphous phase, unstable @ RT by rapid removal of solvent or rapid cooling of melt <sup>[2]</sup>
T <sub>dec.</sub> [°C]	420 K <sup>[1]</sup> , 431 K (mass loss begins, TGA, 3.8 mg sample, @ 10 K/min, N <sub>2</sub> atmosphere, vigorous mass loss @ 470 K) <sup>[1]</sup> , thermal dec. of DATH is highly influenced by heating rate used <sup>[1]</sup> , begins @ 15 K above the mpt. @ 15 psi <sup>[1]</sup>
$\rho$ [g cm <sup>-3</sup> ]	1.72 (X-ray @ 295 K) <sup>[1]</sup>
Heat of formation	148 kcal/mol <sup>[1]</sup>
	Calcd. (EXPLO5 6.03)
	Lit. values
	Exptl.

$-\Delta_{\text{ex}}U^{\circ}$ [kJ kg <sup>-1</sup> ]			
$T_{\text{ex}}$ [K]			
$p_{\text{C},\text{l}}$ [kbar]			
VoD [m s <sup>-1</sup> ]			
$V_0$ [L kg <sup>-1</sup> ]			
Solubility [g/mL]	Recryst. from acetone or CH <sub>3</sub> CN <sup>[1]</sup>		
$\Delta H_{\text{melt}}$ [J/g]	9.7 ± 0.2 kcal/mol (DTA, 1–2 mg sample, @ 5 K/min) <sup>[1]</sup>		

	DATH <sup>[1]</sup>
Chemical formula	C <sub>4</sub> H <sub>8</sub> N <sub>12</sub> O <sub>6</sub>
Molecular weight [g mol <sup>-1</sup> ]	
Crystal system	Triclinic
Space group	P-1
<i>a</i> [Å]	6.407(1)
<i>b</i> [Å]	9.793(2)
<i>c</i> [Å]	10.801(2)
$\alpha$ [°]	109.52(1)
$\beta$ [°]	102.19(1)
$\gamma$ [°]	92.27(1)
<i>V</i> [Å <sup>3</sup> ]	619.8(2)
<i>Z</i>	2
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.72
<i>T</i> [K]	295

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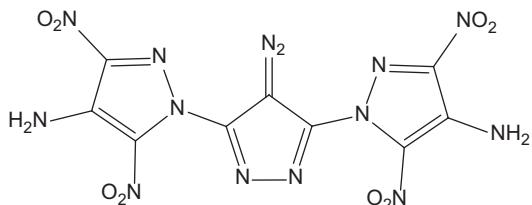
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## 4-Diazo-3,5-bis(4-amino-3,5-dinitropyrazol-1-yl) pyrazole

Name [German, acronym]: 4'-Diazo-3,3<sup>2</sup>,5,5<sup>2</sup>-tetranitro-4'H-[1,3':5',1<sup>2</sup>-terpyrazole]-4,4\*\*-diamine, [LLM-226]

Main (potential) use: Possible future thermally stable insensitive explosive<sup>[1]</sup>

Structural formula:



	LLM-226		
Formula	C <sub>9</sub> H <sub>4</sub> N <sub>14</sub> O <sub>8</sub>		
Molecular mass [g mol <sup>-1</sup> ]	436.22		
Appearance at RT	Pale yellow solid <sup>[1]</sup> , colorless crystals <sup>[1]</sup>		
IS [J]	DH <sub>50</sub> = 31 cm (cf. HMX = 32 cm, 2.5 kg mass, Bruceton method) <sup>[1]</sup>		
FS [N]	1/10 @ 32.4 kg (BAM) <sup>[1]</sup>		
ESD [J]	0.014 @ 0 Ω <sup>[1]</sup>		
N [%]	44.95		
Ω(CO <sub>2</sub> ) [%]	-44.0		
T <sub>m.p.</sub> [°C]	No mpt. in DSC <sup>[1]</sup>		
T <sub>dec.</sub> [°C]	278 (exo peak max., DSC) <sup>[1]</sup>		
ρ [g cm <sup>-3</sup> ]	1.83 <sup>[1]</sup>		
Heat of formation			
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
-Δ <sub>ex</sub> U <sup>o</sup> [kJ kg <sup>-1</sup> ]			
T <sub>ex</sub> [K]			
p <sub>C-J</sub> [kbar]			
VoD [m s <sup>-1</sup> ]			
V <sub>0</sub> [L kg <sup>-1</sup> ]			

	<b>LLM-226<sup>[1]</sup></b>
Chemical formula	C <sub>9</sub> H <sub>4</sub> N <sub>14</sub> O <sub>8</sub>
Molecular weight [g mol <sup>-1</sup> ]	436
Crystal system	Monoclinic
Space group	C2/c
<i>a</i> [Å]	17.869
<i>b</i> [Å]	10.7483
<i>c</i> [Å]	17.307
$\alpha$ [°]	90
$\beta$ [°]	111.099
$\gamma$ [°]	90
<i>V</i> [Å <sup>3</sup> ]	3,101.2
<i>Z</i>	8
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.833
<i>T</i> [K]	20 °C

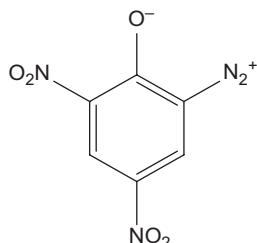
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## 2-Diazonium-4,6-dinitrophenolate

Name [German, acronym]: 2-Diazonium-4,6-dinitrophenolate, diazodinitrophenol, 4,6-dinitrobenzene-2-diazo-1-oxide [DDNP, Dinol, Diazol, DADNP, DIAZ, DADNPh]

Main (potential) use: Primary explosive, commercial blasting caps<sup>[5,15,22]</sup>, in some countries as initiating explosive in military and commercial detonators in past<sup>[14]</sup>, stab and percussion primer mixtures in past<sup>[14]</sup>, as lead-free primer<sup>[14,29]</sup>, component of primer mixtures and as an initiator<sup>[18]</sup>, used as substitute for mercury fulminate<sup>[18]</sup>, percussion caps<sup>[21]</sup>, to a lesser extent in military priming compositions and detonators<sup>[22]</sup>, LA replacement in commercial blasting caps in China<sup>[25]</sup>, LS replacement in nontoxic SINTOX stab mix in commercial impact primers<sup>[25]</sup>

Structural formula:



	<b>DDNP</b>
Formula	C <sub>6</sub> H <sub>2</sub> N <sub>4</sub> O <sub>5</sub>
Molecular mass [g mol <sup>-1</sup> ]	210.10
Appearance at RT	Yellow crystals <sup>[14]</sup> , technical product ranges in color from dark yellow to dark green to dark brown <sup>[14]</sup> , dark brown granular solid <sup>[15]</sup> , yellow amorphous powder if recryst. from acetone by adding large amount of ice water <sup>[15]</sup> , yellow-brown noncrystalline powder or granular material <sup>[18]</sup> , bright yellow crystals or amorphous powder or granules <sup>[20]</sup> , yellow needles <sup>[21]</sup> , greenish yellow-brown solid with tabular crystals <sup>[5]</sup> , greenish-yellow to brown solid <sup>[22]</sup> , reddish-yellow amorphous powder <sup>[29]</sup>

IS [J]	<p>1 (100–500 µm), 1.5 Nm<sup>[2,4]</sup>, less sensitive than LA or MF<sup>[5]</sup>, <math>H_{50\%} = 9.4</math> cm (2 kg mass, type 12 tool, B.M.)<sup>[7]</sup>, <math>H_{50\%} = 9</math> cm (2.5 kg mass, type 12 tool, B.M., 35 mg sample, garnet paper)<sup>[8]</sup>, highly particle size dependent<sup>[14]</sup>, ~0.8 (P.A.)<sup>[14]</sup>, ~1.1<sup>[14]</sup>, less sensitive than mercury fulminate or Pb(N<sub>3</sub>)<sub>2</sub><sup>[15]</sup>, 4 in (2 kg mass, 20 mg sample, P.A.)<sup>[21]</sup>, 7 in (1 lb mass, 15 mg sample, P.A.)<sup>[21]</sup>, 1<sup>[30]</sup>, 40 cm (100% fire, 400 g hammer, 20 mg sample)<sup>[31]</sup>, 17.5 cm (100% no fire, 400 g hammer 20 mg sample)<sup>[31]</sup></p> <p>Impact initiation delay, delay range is for approx. 20 initiations<sup>[32]</sup>:</p> <table border="1"> <thead> <tr> <th>Impact energy (J)</th><th>Average delay (µs)</th><th>Delay range (µs)</th></tr> </thead> <tbody> <tr> <td>6.34</td><td>277</td><td>80–235</td></tr> <tr> <td>4.85</td><td>361</td><td>80–620</td></tr> <tr> <td>3.40</td><td>425</td><td>180–1,335</td></tr> <tr> <td>1.94</td><td>494</td><td>240–680</td></tr> <tr> <td>0.98</td><td>274</td><td>100–620</td></tr> </tbody> </table> <p>Effect of liquid nitrogen on the IS (2 kg mass, modified P.A. machine, 50% point, <math>T</math> cycling = soaking sample in LN<sub>2</sub> for 15 min then allowing to stand at ambient <math>T</math> for 1 h for five cycles)<sup>[32]</sup>:</p> <table border="1"> <thead> <tr> <th></th><th>Height (cm) (standard deviation)</th></tr> </thead> <tbody> <tr> <td colspan="2">Mean height for 50% probability of reaction</td></tr> <tr> <td>Control (dry)</td><td>9.65 (4.10)</td></tr> <tr> <td>LN<sub>2</sub> test</td><td>9.27 (2.72)</td></tr> <tr> <td colspan="2">Height for 10% probability of reaction</td></tr> <tr> <td>Control (dry)</td><td>5.08</td></tr> <tr> <td>LN<sub>2</sub> test</td><td>5.08</td></tr> <tr> <td colspan="2">Effect of <math>T</math> cycling at 50% height</td></tr> <tr> <td>In LN<sub>2</sub>, % fire</td><td>45</td></tr> <tr> <td>Dry, % fire</td><td>35</td></tr> </tbody> </table>	Impact energy (J)	Average delay (µs)	Delay range (µs)	6.34	277	80–235	4.85	361	80–620	3.40	425	180–1,335	1.94	494	240–680	0.98	274	100–620		Height (cm) (standard deviation)	Mean height for 50% probability of reaction		Control (dry)	9.65 (4.10)	LN <sub>2</sub> test	9.27 (2.72)	Height for 10% probability of reaction		Control (dry)	5.08	LN <sub>2</sub> test	5.08	Effect of $T$ cycling at 50% height		In LN <sub>2</sub> , % fire	45	Dry, % fire	35
Impact energy (J)	Average delay (µs)	Delay range (µs)																																					
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In LN <sub>2</sub> , % fire	45																																						
Dry, % fire	35																																						
FS [N]	<p>5 (100–500 µm), 20<sup>[2]</sup>, 22<sup>[3]</sup>, similar to LA<sup>[5]</sup>, 436 lb (ABL, 50% load, pendulum friction test)<sup>[7]</sup>, 2.99 (50% initiation probability)<sup>[14]</sup>, <math>F_{50} = 21.5</math> (dry sample) (FSKM-PEx OZM friction tester, roughened ceramic plate and porcelain peg)<sup>[17]</sup>, <math>F_{50} = 22.43</math> (5% water) (FSKM-PEx OZM friction tester, roughened ceramic plate and porcelain peg)<sup>[17]</sup>, <math>F_{50} = 30.55</math> (10% water) (FSKM-PEx OZM friction tester, roughened ceramic plate and porcelain peg)<sup>[17]</sup>, <math>F_{50} = 46.1</math> (20% water) (FSKM-PEx OZM friction tester, roughened ceramic plate and porcelain peg)<sup>[17]</sup>, <math>F_{50} = 44.97</math> (excess water) (FSKM-PEx OZM friction tester, roughened ceramic plate and porcelain peg)<sup>[17]</sup>, detonates with steel shoe (friction pendulum test)<sup>[21]</sup>, detonates with fiber shoe (friction pendulum test)<sup>[21]</sup>, 24.7<sup>[30]</sup>, 25% (explosion % of 25 samples under 588.40 kPa and 80° swing angle)<sup>[31]</sup></p>																																						

	Yamada friction apparatus <sup>[32]</sup> :				
	DDNP particle size (mm)	Additive	Load for 50% initiations (kg)		
			Emery	Ebonite	Copper
0.3–0.5	—		15.0	52.0	MOO
	Ground glass 100 mesh		12.5	27.0	32.0
ESD [J]	0.15 (100–500 µm), max. energy of static discharge that does not cause ignition = 0.25 <sup>[5]</sup> , 0.09 (ERL) <sup>[7]</sup> , 1.8 m <sup>[14,30]</sup> , 0.012 <sup>[21,31]</sup>  Highest electrostatic discharge energy @ 5000 volts for zero ignition probability <sup>[9]</sup> :				
	Highest energy (J) for zero ignition probability	Type of ignition			
	Unconfined	Confined	Unconfined	Confined	
	0.012	0.012	None	Deflagration	
N [%]	26.67				
Ω(CO <sub>2</sub> ) [%]	−60.92				
T <sub>m.p.</sub> [°C]	Decomposes without melting, 157 (melts then dec., capillary tube) <sup>[7]</sup> , ~435 K (DSC @ 20 K/min) <sup>[7]</sup> , 157–158 (dec.) <sup>[14]</sup> , 157 <sup>[18,21,22,23]</sup> , 160 (dec.) <sup>[29]</sup>				
T <sub>dec.</sub> [°C]	163 (ignition temperature ~172 °C <sup>[1]</sup> , DSC @ 5 °C/min) <sup>[1]</sup> , 157 <sup>[30]</sup>				
ρ [g cm <sup>−3</sup> ]	1.727 (@ 295 K), 1.726 (@ 298 K, calcd.), 1.63 (crystal) <sup>[2,23]</sup> , 1.63–1.65 (crystal @ 25 °C) <sup>[5]</sup> , 1.63 (technical product) <sup>[14]</sup> , 1.719 (crystal, X-ray) <sup>[14]</sup> , 0.5–0.9 (bulk ρ) <sup>[14]</sup> , 0.27 (fine powder ρ) <sup>[14]</sup> , 1.63 (true ρ @ 25 °/4 °) <sup>[15]</sup> , 0.27 (apparent ρ after being placed in tube and tapped) <sup>[15]</sup> , 0.86 (apparent ρ after being compressed in a detonator capsule at a pressure of 3400 lb/in <sup>2</sup> <sup>[15]</sup> , 1.63 (crystal) <sup>[21]</sup> , 0.27 (apparent density) <sup>[21]</sup> , 1.14 (@ 3000 psi) <sup>[21]</sup> , 1.71 (crystal) <sup>[25]</sup> , 1.63 <sup>[29]</sup> , 1.7 <sup>2</sup> <sup>[30]</sup>				
Heat of formation	988.9 kJ/kg (energy of form.) <sup>[4]</sup> , 924.0 kJ/kg (enthalpy of form.) <sup>[4]</sup> , 956 cal/g <sup>[5]</sup> , 321 kJ/mol <sup>[14]</sup> , 194 kJ/mol (enthalpy of form.) <sup>[29]</sup> , 321 kJ/mol (Δ <sub>f</sub> H) <sup>[30]</sup> , 46.39 kcal/mol (ΔH <sub>f</sub> <sup>o</sup> ) <sup>[33]</sup>				
Heat of combustion	3,243 kcal/kg <sup>[10,21,23]</sup>				
	Calcd. (EXPLO5 6.03)	Lit. values		Expl.	

$-\Delta_{\text{ex}}U^{\circ} [\text{kJ kg}^{-1}]$	4,604	820 kcal/kg <sup>[10]</sup>	820 cal/g <sup>[5,21,23]</sup>
$T_{\text{ex}} [\text{K}]$	3,559		
$p_{\text{C-J}} [\text{kbar}]$	219	24.2 GPa (calcd.) <sup>[30]</sup>	
VoD [m s <sup>-1</sup> ]	7,331 (@ TMD)	7,220 (@ 1.63 g cm <sup>-3</sup> (TMD), calcd., R-P method) <sup>[11]</sup>  4,400 (@ 0.9 g cm <sup>-3</sup> ) <sup>[14]</sup>  6,600 (@ 1.5 g cm <sup>-3</sup> ) <sup>[14]</sup>  6,900 (@ 1.6 g cm <sup>-3</sup> ) <sup>[14,30]</sup>	~6,900 (@ 1.6 g cm <sup>-3</sup> ) <sup>[1,2,25]</sup>  6,900 (@ 1.6 g cm <sup>-3</sup> ) <sup>[13]</sup>  6,900 (@ 1.58 g cm <sup>-3</sup> ) <sup>[5]</sup>  7,100 (@ 1.63 g cm <sup>-3</sup> ) <sup>[5]</sup>  4,100 (@ 0.9 g cm <sup>-3</sup> ) <sup>[5]</sup>  6,600 (@ 1.5 g cm <sup>-3</sup> ) <sup>[4]</sup>  22,600 ft/s (@ 1.6 g/mL) <sup>[18]</sup>  4,400 (@ 0.9 g cm <sup>-3</sup> , pressed) <sup>[21]</sup>  6,600 (@ 1.5 g cm <sup>-3</sup> , pressed) <sup>[21]</sup>  6,900 (@ 1.6 g cm <sup>-3</sup> , pressed) <sup>[21]</sup>
$V_0 [\text{L kg}^{-1}]$	629		856 <sup>[5]</sup>  865 <sup>[21,23]</sup>
$I_{\text{sp}} [\text{Ns g}^{-1}]$	2.27 (calcd., ISPBKW code) <sup>[33]</sup> , 2.23 (calcd., empirical) <sup>[33]</sup>		

Trauzl test [cm <sup>3</sup> , % TNT]	110% TNT <sup>[5]</sup> , 25.0 cm <sup>3</sup> <sup>[14]</sup> , 25 cc (1 g DDNP in a No. 8 detonator capsule compressed under a reenforcing cap at a pressure of 3,400 lb/in <sup>2</sup> and fired in a small Trauzl block) <sup>[15]</sup> , 13.4 cc (small Trauzl test) <sup>[19]</sup> , rel. strength cf. TNT = 1.10 <sup>[19]</sup> , 326 <sup>[27]</sup>
Lead block compression test	10.5 mm shortening of block (small lead block compression test, 50 g DDNP exploded by means of detonator on top of a cylinder 64 mm long) <sup>[15]</sup>
Sand test [g]	97–105% TNT <sup>[5]</sup> , 94–105% TNT <sup>[5]</sup> , 19.3 g sand crushed (0.2 g charge measured in detonator shell, pressed under a reinforcing capsule @ 23.4 MPa) <sup>[14]</sup> , 90.6 g sand crushed (1.0 g charge measured in detonator shell, pressed under a reinforcing capsule @ 23.4 MPa) <sup>[14]</sup> , 47.5 g (200 g bomb) <sup>[21]</sup>

	<p>Weight of sand pulverized (g) by DDNP (g) (no. 8 detonator capsules, pressed under reinforcing caps at 3,400 lb/in<sup>2</sup>, fired in no. 2 sand test bomb)<sup>[15]</sup>:</p> <table border="1"> <thead> <tr> <th>Weight of DDNP charge (g)</th><th>Weight of sand pulverized (g)</th></tr> </thead> <tbody> <tr><td>0.10</td><td>9.1</td></tr> <tr><td>0.20</td><td>19.3</td></tr> <tr><td>0.40</td><td>36.2</td></tr> <tr><td>0.60</td><td>54.3</td></tr> <tr><td>0.80</td><td>72.1</td></tr> <tr><td>1.00</td><td>90.5</td></tr> </tbody> </table> <p>63.9 g (amount of sand crushed finer than 30 mesh, by total charge consisting of base charge of 0.50 g DDNP and 0.30 g priming charge of MF)<sup>[19]</sup>, 52.2 g (amount of sand crushed finer than 30 mesh, by base charge of 0.50 g DDNP)<sup>[19]</sup>, rel. strength cf. TNT = 1.20<sup>[19]</sup></p>	Weight of DDNP charge (g)	Weight of sand pulverized (g)	0.10	9.1	0.20	19.3	0.40	36.2	0.60	54.3	0.80	72.1	1.00	90.5																									
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Ballistic mortar test	95% TNT <sup>[5]</sup> , 97% TNT <sup>[21]</sup>																																							
Initiating efficiency	<p>0.12 g initiates tetryl<sup>[14]</sup>, 0.15 g initiates TNT<sup>[14]</sup>, 0.28 g initiates ammonium picrate<sup>[14]</sup>, max. initiation efficiency @ <math>\rho = 1.2\text{--}1.3 \text{ g cm}^{-3}</math><sup>[14]</sup></p> <p>Influence of compacting pressure and specific surface on initiation efficiency (acceptor = 0.35 g TNT compressed by 76.5 MPa with reinforcing cap)<sup>[14]</sup>:</p> <table border="1"> <thead> <tr> <th>Specific surface (cm<sup>2</sup>/g)</th><th>Compacting pressure (MPa)</th><th>Min. amount DDNP (g)</th></tr> </thead> <tbody> <tr> <td rowspan="4">6,840</td><td>~ 1</td><td>~ 0.21</td></tr> <tr><td>~ 14</td><td>~ 0.11</td></tr> <tr><td>~ 29</td><td>~ 0.21</td></tr> <tr><td>~ 35</td><td>~ 0.275</td></tr> <tr> <td rowspan="4">3,360</td><td>~ 1</td><td>~ 0.14</td></tr> <tr><td>~ 14</td><td>~ 0.09</td></tr> <tr><td>~ 29</td><td>~ 0.14</td></tr> <tr><td>~ 35</td><td>~ 0.245</td></tr> <tr> <td rowspan="4">2,253</td><td>~ 1</td><td>~ 0.12</td></tr> <tr><td>~ 14</td><td>~ 0.12</td></tr> <tr><td>~ 29</td><td>~ 0.11</td></tr> <tr><td>~ 35</td><td>~ 0.22</td></tr> <tr> <td rowspan="4">4,750</td><td>~ 1</td><td>~ 0.12</td></tr> <tr><td>~ 14</td><td>~ 0.09</td></tr> <tr><td>~ 29</td><td>~ 0.165</td></tr> <tr><td>~ 35</td><td>~ 0.25</td></tr> </tbody> </table>	Specific surface (cm <sup>2</sup> /g)	Compacting pressure (MPa)	Min. amount DDNP (g)	6,840	~ 1	~ 0.21	~ 14	~ 0.11	~ 29	~ 0.21	~ 35	~ 0.275	3,360	~ 1	~ 0.14	~ 14	~ 0.09	~ 29	~ 0.14	~ 35	~ 0.245	2,253	~ 1	~ 0.12	~ 14	~ 0.12	~ 29	~ 0.11	~ 35	~ 0.22	4,750	~ 1	~ 0.12	~ 14	~ 0.09	~ 29	~ 0.165	~ 35	~ 0.25
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Influence of  $\rho$  of DDNP and specific surface on initiation efficiency  
(acceptor = 0.35 g TNT compressed by 76.5 MPa with reinforcing cap)<sup>[14]</sup>:

Specific surface (cm <sup>2</sup> /g)	$\rho$ (g cm <sup>-3</sup> )	Min. amount DDNP (g)
6,840	~ 0.7	~ 0.215
	~ 1.3	~ 0.105
	~ 1.39	~ 0.215
	~ 1.41	~ 0.279
	~ 1.44	~ 0.29
2,253	~ 0.39	~ 0.12
	~ 1.15	~ 0.115
	~ 1.4	~ 0.115
	~ 1.5	~ 0.219
	~ 1.55	~ 0.25
4,750	~ 0.55	~ 0.11
	~ 1.22	~ 0.095
	~ 1.34	~ 0.245
	~ 1.38	~ 0.29

$\rho$  of DDNP as function of compacting pressure on initiation efficiency  
(specific surface = 2,253 cm<sup>2</sup>/g; acceptor = 0.35 g TNT)<sup>[14]</sup>:

Compacting pressure (MPa)	$\rho$ (g/cm <sup>3</sup> )	Compacting pressure (MPa)	$\rho$ (g/cm <sup>3</sup> )
0	~ 0.3	~ 58	~ 1.50
10	~ 1.0	~ 70	~ 1.50
20	~ 1.25	~ 81	~ 1.52
30	~ 1.4	~ 90	~ 1.55
40	~ 1.45	100	~ 1.6
~ 50	~ 1.45	~ 121	~ 1.65

Does not explode under water using a no. 8 blasting cap<sup>[15,18]</sup>

Minimum initiating charge of DDNP needed for high explosive (0.5 g charges of H.E. in no. 8 detonator capsule, with reinforcement caps, charges compressed under pressure of 3,400 lb/in<sup>2</sup>)<sup>[15]</sup>: 0.115 g for picric acid, 0.163 g for TNT, 0.075 g for tetryl, 0.110 g for trinitroresorcinol, 0.075 g for trinitrobenzaldehyde, 0.085 g for tetranitroaniline, 0.075 g for hexanitrodiphenylamine, 0.05 for pentryl, without reinforcing cap DDNP did not cause detonation<sup>[15]</sup>

	<p>Cannot be detonated underwater with a no. 8 electric detonator<sup>[20]</sup>, 0.20 g LA minimum detonating charge<sup>[21]</sup>, 0.10 g tetryl minimum detonating charge<sup>[21]</sup></p> <p>Efficiency of initiating compounds<sup>[5]</sup>:</p> <table border="1"> <thead> <tr> <th></th><th colspan="3">Minimum detonating charge, g of initiator required to detonate</th></tr> <tr> <th></th><th>Tetryl</th><th>TNT</th><th>Ammonium picrate</th></tr> </thead> <tbody> <tr> <td>Lead azide</td><td>0.10</td><td>0.26</td><td>No detonation</td></tr> <tr> <td>Mercury fulminate</td><td>0.19</td><td>0.24</td><td>No detonation</td></tr> <tr> <td>Diazodinitrophenol</td><td>0.12</td><td>0.15</td><td>0.28</td></tr> </tbody> </table> <p>MPC = 70 mg (minimum primary charge), AC = 230–280 mg (actual charge)<sup>[30]</sup></p>		Minimum detonating charge, g of initiator required to detonate				Tetryl	TNT	Ammonium picrate	Lead azide	0.10	0.26	No detonation	Mercury fulminate	0.19	0.24	No detonation	Diazodinitrophenol	0.12	0.15	0.28
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Dead-pressing	<p>Not dead-pressed even @ 13,000 lb/in<sup>2[5]</sup>, not dead-pressed up to 690 MPa (old lit. values)<sup>[14]</sup>, completely dead-pressed @ <math>\rho = 1.4 \text{ g cm}^{-3}</math><sup>[14]</sup>, dead-pressed @ pressures &gt;19.6 MPa<sup>[14]</sup>, max. initiation efficiency @ <math>\rho = 1.2\text{--}1.3 \text{ g cm}^{-3}</math><sup>[14]</sup>, not dead-pressed by a pressure of 130,000 lb/in<sup>2[5]</sup>, does not get dead-pressed<sup>[20]</sup>, pressure durability = &lt;60 MPa (later this value DDNP is dead-pressed)<sup>[30]</sup></p>																				
5 s explosion $T$ [°C] 1 s explosion $T$ [°C] 5 s ignition $T$ [°C] Ignition $T$ [°C]  Explosion $T$ [°C]	<p>195<sup>[5,21,22]</sup>, 172<sup>[31]</sup> 200<sup>[14,15,21]</sup></p> <p>195 (explodes, USA)<sup>[10]</sup>, 180 (Russian value<sup>[10]</sup>), 185<sup>[14,15]</sup>, 177<sup>[14]</sup> 157 (heating in glass tube @ 5 °C/min)<sup>[7]</sup>, 161–163 (@ 5 °C/min, static air atmosphere, DDNP prepared by Garfield's method)<sup>[14]</sup>, ~ 172<sup>[25]</sup>, 164<sup>[28]</sup></p> <p>Explosion <math>T</math> @ various times of exposure (3 mg sample, detonation)<sup>[12]</sup>:</p> <table border="1"> <thead> <tr> <th><math>T</math> (°C)</th> <th>Time (s)</th> </tr> </thead> <tbody> <tr> <td>247</td> <td>0.133</td> </tr> <tr> <td>200</td> <td>0.725</td> </tr> <tr> <td>177</td> <td>5.00</td> </tr> <tr> <td>168</td> <td>16</td> </tr> <tr> <td>160</td> <td>No action</td> </tr> </tbody> </table> <p>10 s explosion time @ 180 °C (0.02 g DDNP dropped onto a heated bath of molten metal)<sup>[15]</sup>, 2.5 s explosion time @ 190 °C (0.02 g DDNP dropped onto a heated bath of molten metal)<sup>[15]</sup>, dec. without explosion @ 177 °C (0.02 g DDNP dropped onto a heated bath of molten metal)<sup>[15]</sup>, 180<sup>[20]</sup>, 180 (10 s)<sup>[21]</sup></p> <p>Detonating <math>T</math> [°C]</p> <p>195<sup>[18]</sup></p>	$T$ (°C)	Time (s)	247	0.133	200	0.725	177	5.00	168	16	160	No action								
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100 °C heat test [% mass loss]	2.1% mass loss in first 48 h <sup>[5,21]</sup> , 2.2% mass loss in second 48 h <sup>[5,21]</sup> , no explosions during 100 h <sup>[5,21]</sup> , 1.25% mass loss after 96 h @ 100 °C <sup>[14]</sup>																																																										
Vacuum stability test [cm <sup>3</sup> /h]	7.6 cm <sup>3</sup> gas evolved @ 100 °C from 5 g sample in 40 h <sup>[5,21]</sup>																																																										
Thermal stability	Dry DDNP withstands storage @ 50 °C for at least 30 months <sup>[5,22]</sup> , if stored underwater no decrease in its brisance is observed after 24 months @ RT <sup>[5]</sup> , or @ 50 °C for 12 months underwater <sup>[5]</sup> , no change on storing @ 65 °C <sup>[14]</sup> , unaffected after 30 months @ 50 °C <sup>[21]</sup>																																																										
Burn rate [mm/s]	Unconfined sample burns with a flash if ignited <sup>[5]</sup> , slight confinement is enough to cause transition from burning to detonation <sup>[5]</sup> Linear and mass rates of burning @ 1 atm <sup>[26]</sup> : $u = 2.15 \text{ cm/s}$ <sup>[26]</sup> , $m = 3.12 \text{ g cm}^{-2} \text{ s}^{-1}$ <sup>[26]</sup>																																																										
Solubility [g/mL]	<p>0.08 g/100 mL H<sub>2</sub>O (@ 25 °C) (slightly soluble in H<sub>2</sub>O)<sup>[14]</sup>, soluble (recryst.) in hot acetone and nitrobenzene<sup>[14]</sup>, soluble in NG, nitrobenzene, aniline, pyridine, conc. HCl, and in most common organic solvents<sup>[21]</sup></p> <p>Solubilities in organic solvents<sup>[14]</sup>:</p> <table border="1"> <thead> <tr> <th rowspan="2">Solvent</th> <th colspan="2">Solubility (g/100 g solvent)</th> <th rowspan="2">Solvent</th> <th colspan="2">Solubility (g/100 g solvent)</th> </tr> <tr> <th>25 °C</th> <th>50 °C</th> <th>25 °C</th> <th>50 °C</th> </tr> </thead> <tbody> <tr> <td>H<sub>2</sub>O</td> <td>0.08</td> <td>—</td> <td>Toluene</td> <td>—</td> <td>0.15</td> </tr> <tr> <td>Ethyl acetate</td> <td>—</td> <td>2.45</td> <td>Petrol ether</td> <td>—</td> <td>—</td> </tr> <tr> <td>Methanol</td> <td>0.57</td> <td>1.25</td> <td>Ethyl ether</td> <td>0.04</td> <td>0.08 (@ 30 °C)</td> </tr> <tr> <td>Ethanol</td> <td>0.84</td> <td>2.43</td> <td>CS<sub>2</sub></td> <td>—</td> <td>trace (@ 30 °C)</td> </tr> <tr> <td>CCl<sub>4</sub></td> <td>—</td> <td>Trace</td> <td>Acetic acid</td> <td>1.40</td> <td>—</td> </tr> <tr> <td>Benzene</td> <td>0.09</td> <td>0.23</td> <td>Acetone</td> <td>6.0</td> <td>—</td> </tr> </tbody> </table> <p>Solubility in organic solvents @ 50 °C<sup>[15]</sup>:</p> <table border="1"> <thead> <tr> <th>Solvent</th> <th>Solubility (g) in 100 g solvent @ 50 °C</th> </tr> </thead> <tbody> <tr> <td>Ethyl acetate</td> <td>2.45</td> </tr> <tr> <td>MeOH</td> <td>1.25</td> </tr> <tr> <td>EtOH</td> <td>2.43</td> </tr> <tr> <td>Benzene</td> <td>0.23</td> </tr> <tr> <td>CHCl<sub>3</sub></td> <td>0.11</td> </tr> </tbody> </table>	Solvent	Solubility (g/100 g solvent)		Solvent	Solubility (g/100 g solvent)		25 °C	50 °C	25 °C	50 °C	H <sub>2</sub> O	0.08	—	Toluene	—	0.15	Ethyl acetate	—	2.45	Petrol ether	—	—	Methanol	0.57	1.25	Ethyl ether	0.04	0.08 (@ 30 °C)	Ethanol	0.84	2.43	CS <sub>2</sub>	—	trace (@ 30 °C)	CCl <sub>4</sub>	—	Trace	Acetic acid	1.40	—	Benzene	0.09	0.23	Acetone	6.0	—	Solvent	Solubility (g) in 100 g solvent @ 50 °C	Ethyl acetate	2.45	MeOH	1.25	EtOH	2.43	Benzene	0.23	CHCl <sub>3</sub>	0.11
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	<p>Soluble in nitrobenzene, acetone, aniline, pyridine, acetic acid, NG at RT<sup>[15]</sup>, slightly soluble in EtOH and ethyl acetate<sup>[18]</sup>, soluble in acetone and nitrobenzene<sup>[18]</sup></p> <p>Solubility: g DDNP/100 g solvent @ 50 °C<sup>[21]</sup>:</p> <table border="1"> <thead> <tr> <th>Solvent</th><th>%</th><th>Solvent</th><th>%</th></tr> </thead> <tbody> <tr> <td>Ethyl acetate</td><td>2.45</td><td>CHCl<sub>3</sub></td><td>0.11</td></tr> <tr> <td>Methanol</td><td>1.25</td><td>Benzene</td><td>0.23</td></tr> <tr> <td>Ethanol</td><td>2.43</td><td>Toluene</td><td>0.15</td></tr> <tr> <td>Ethylenedichloride</td><td>0.79</td><td>Petroleum ether</td><td>Insoluble (@ 20 °C)</td></tr> <tr> <td>CCl<sub>4</sub></td><td>Trace</td><td>Et<sub>2</sub>O</td><td>0.08 (@ 30 °C)</td></tr> <tr> <td>CS<sub>2</sub></td><td>Trace (@ 30 °C)</td><td></td><td></td></tr> </tbody> </table> <p>Data from ref.<sup>[5]</sup></p> <table border="1"> <thead> <tr> <th rowspan="2">Solvent</th><th colspan="2">g DDNP/100 g solvent</th></tr> <tr> <th>@ 25 °C</th><th>@ 50 °C</th></tr> </thead> <tbody> <tr> <td>Water</td><td>0.08</td><td>–</td></tr> <tr> <td>Benzene</td><td>0.09</td><td>0.23</td></tr> <tr> <td>MeOH</td><td>0.57</td><td>1.25</td></tr> <tr> <td>EtOH</td><td>0.84</td><td>2.43</td></tr> <tr> <td>Et<sub>2</sub>O</td><td>0.04</td><td>–</td></tr> <tr> <td>CHCl<sub>3</sub></td><td>–</td><td>0.11</td></tr> <tr> <td>Ethylene chloride</td><td>0.29</td><td>–</td></tr> <tr> <td>Acetic acid</td><td>1.40</td><td>–</td></tr> <tr> <td>Ethyl acetate</td><td>–</td><td>2.45</td></tr> <tr> <td>Acetone</td><td>6.0</td><td>–</td></tr> </tbody> </table> <p>Some solubility in NG, nitrobenzene, aniline, pyridine and conc. HCl<sup>[5]</sup>, almost insoluble in CS<sub>2</sub> and CCl<sub>4</sub><sup>[5]</sup></p>	Solvent	%	Solvent	%	Ethyl acetate	2.45	CHCl <sub>3</sub>	0.11	Methanol	1.25	Benzene	0.23	Ethanol	2.43	Toluene	0.15	Ethylenedichloride	0.79	Petroleum ether	Insoluble (@ 20 °C)	CCl <sub>4</sub>	Trace	Et <sub>2</sub> O	0.08 (@ 30 °C)	CS <sub>2</sub>	Trace (@ 30 °C)			Solvent	g DDNP/100 g solvent		@ 25 °C	@ 50 °C	Water	0.08	–	Benzene	0.09	0.23	MeOH	0.57	1.25	EtOH	0.84	2.43	Et <sub>2</sub> O	0.04	–	CHCl <sub>3</sub>	–	0.11	Ethylene chloride	0.29	–	Acetic acid	1.40	–	Ethyl acetate	–	2.45	Acetone	6.0	–
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Hygroscopicity	Very slightly hygroscopic <sup>[14]</sup> , 1% mass gain on storing for 40 days @ 70% humidity <sup>[14]</sup> , 2.25% mass gain on storing @ 100% humidity <sup>[14]</sup> , 0.04 % mass gain on storing @ 30 °C @ 90% humidity <sup>[14]</sup> , slightly hygroscopic – does not react with H <sub>2</sub> O @ RT but is desensitized by it <sup>[18]</sup> , 0.04% @ 30 °C with 90% RH <sup>[5,21]</sup> , not hygroscopic <sup>[22]</sup>																																																															
Photosensitivity	Darkens on irradiation by light <sup>[14,30]</sup> , partial dec. after 40 h in sunlight <sup>[14]</sup> , darkens rapidly on exposure to sunlight <sup>[15,18]</sup> , rapidly darkens on exposure to light <sup>[5]</sup> , unstable on exposure to light <sup>[25]</sup>																																																															

Radiation sensitivity	<p>Data obtained for explosives after exposure to gamma radiation<sup>[23]</sup>:</p> <table border="1" data-bbox="354 206 965 918"> <tbody> <tr> <td>Weight of sample (g)</td><td>2</td></tr> <tr> <td>Vol. of gas produced (mL/g) in following times (days)</td><td></td></tr> <tr> <td>10</td><td>0.25</td></tr> <tr> <td>20</td><td>1.55</td></tr> <tr> <td>30</td><td>3.25</td></tr> <tr> <td>40</td><td>5.60</td></tr> <tr> <td>50</td><td>7.2</td></tr> <tr> <td>90</td><td>-</td></tr> <tr> <td>Total irradiation time (days)</td><td>45</td></tr> <tr> <td>IS (P.A. apparatus) (in)</td><td></td></tr> <tr> <td>Original material</td><td>2</td></tr> <tr> <td>Irradiated material</td><td>2</td></tr> <tr> <td>IS (B.M. apparatus) (cm)*</td><td></td></tr> <tr> <td>Original material</td><td>4</td></tr> <tr> <td>Irradiated material</td><td>3</td></tr> <tr> <td>Sand test, 200 g bomb, g of sand crushed when sample was ignited by black powder fuse only</td><td></td></tr> <tr> <td>Original material</td><td>22.1</td></tr> <tr> <td>Irradiated material</td><td>14.1</td></tr> </tbody> </table>	Weight of sample (g)	2	Vol. of gas produced (mL/g) in following times (days)		10	0.25	20	1.55	30	3.25	40	5.60	50	7.2	90	-	Total irradiation time (days)	45	IS (P.A. apparatus) (in)		Original material	2	Irradiated material	2	IS (B.M. apparatus) (cm)*		Original material	4	Irradiated material	3	Sand test, 200 g bomb, g of sand crushed when sample was ignited by black powder fuse only		Original material	22.1	Irradiated material	14.1
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Compatibility	Incompatible with lead azide <sup>[14]</sup> , does not react with H <sub>2</sub> O @ RT but is desensitized by it <sup>[15,18]</sup> , reacts slightly with copper and readily with lead azide <sup>[18]</sup>																																				
Blast characteristics	Loose – filled into mild steel test units (4.6 cm × 2.5 cm × 2.5 cm; 0.9 cm hole diameter), sealed with a cork disk and adhesive. Mass of material = 200–1,000 mg, initiated with an ICI Type E fusehead: peak overpressure (blast wave) $p_{\max}$ = 3.6 kPa (mean value) <sup>[16]</sup> standard deviation $\sigma$ = 0.19 kPa <sup>[16]</sup> positive phase impulse (blast wave) $I^+$ = 0.38 Pa s (mean value) <sup>[16]</sup>																																				
Firing times of hot bridgewire initiators	<p>Firing times of hot bridgewire initiator, 50 mg loads of explosives, 450 V voltage, times in <math>\mu</math>s<sup>[23]</sup>:</p> <table border="1" data-bbox="354 1314 837 1426"> <thead> <tr> <th>Milling time (h)</th> <th colspan="3">Capacitance (<math>\mu</math>F)</th> </tr> </thead> <tbody> <tr> <td>0.5</td> <td>0.05</td> <td>0.0047</td> <td></td> </tr> <tr> <td>24</td> <td>8.33–9.00</td> <td>10.0–13.8</td> <td>91.2–362.5</td> </tr> </tbody> </table>	Milling time (h)	Capacitance ( $\mu$ F)			0.5	0.05	0.0047		24	8.33–9.00	10.0–13.8	91.2–362.5																								
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Laser sensitivity	DDNP can be successfully initiated using a UV excimer laser <sup>[24]</sup> :						
	Pressing force (kN)	Detonator type	Nominal wavelength (nm)	Energy density (kJ/m <sup>2</sup> )	Function time (μs)	Source	Pulse duration (μs)
	1	Confined	249	—	15	Excimer laser	15
	10	Confined	249	—	210	Excimer laser	15
Ignition sensitivity by electric bridge current	Bridge current and ignition time ( $I$ = ignition current (ampere), $s$ = ignition time (s), $I^2s$ = (ignition current) <sup>2</sup> × (ignition time)) <sup>[28]</sup> :						
	I	2.0	1.6	1.3	1.0	0.8	
	S	4.1	3.1	6.3	10.1	12.8	
	FS	16.4	13.1	10.7	10.1	8.2	
Flame test	Flame sensitivity $H_{50} \geq 17$ cm ( $H_{50}$ reflects the reliability of ignition) <sup>[30]</sup>						
Flowability	$\theta = 29.01^\circ$ , satisfactory flowability <sup>[30]</sup>						

	DDNP <sup>[6]</sup>	DDNP <sup>[7]</sup>
Chemical formula	C <sub>6</sub> H <sub>2</sub> N <sub>4</sub> O <sub>5</sub>	C <sub>6</sub> H <sub>2</sub> N <sub>4</sub> O <sub>5</sub>
Molecular weight [g mol <sup>-1</sup> ]	210.12	210.12
Crystal system	Orthorhombic	Orthorhombic
Space group	<i>P</i> 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub> (no. 19)	<i>P</i> 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub> (no. 19)
<i>a</i> [Å]	6.1777(7)	6.184(2)
<i>b</i> [Å]	8.605(1)	8.625(3)
<i>c</i> [Å]	15.205(2)	15.222(4)
$\alpha$ [°]	90	90
$\beta$ [°]	90	90
$\gamma$ [°]	90	90
<i>V</i> [Å <sup>3</sup> ]	808.2	811.96(41)
<i>Z</i>	4	4
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.727	1.719
<i>T</i> [K]	295	

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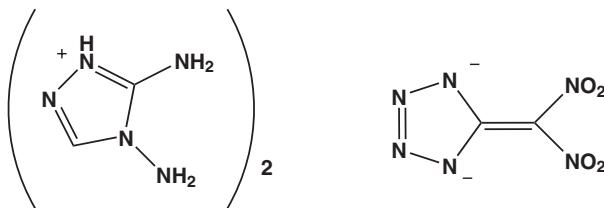
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**Di(3,4-diamino-1,2,4-triazolium) 5-dinitromethyl-tetrazolate**

Name [German, acronym]: Di(3,4-diamino-1,2,4-triazolium) 5-dinitromethyl-tetrazolate [2DATr.DNMZ]

Main (potential) use: Secondary explosive

Structural formula:



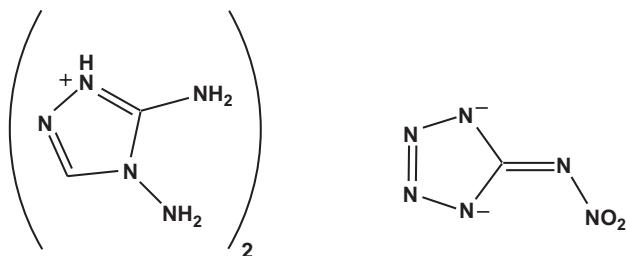
	2DATr.DNMZ	
Formula	$C_6H_{12}N_{16}O_4$ , $[C_2H_6N_5]^+{}_2 [CN_5O_4]^{2-}$	
Molecular mass [g mol <sup>-1</sup> ]	372.12	
Appearance at RT		
IS [J]	37	
N [%]	60.2	
$\Omega(CO_2)$ [%]	-60	
$T_{m.p.}$ [°C]	200	
$T_{dec.}$ [°C]	256 (DSC @ 5 °C/min)	
$\rho$ [g cm <sup>-3</sup> ]	1.629 (@ 296 K), 1.629 (@ 298 K)	
Heat of formation	622.9 kJ/mol ( $\Delta_fH^\circ$ )	
	Calcd. (K-J)	Exptl.
$-\Delta_{ex}U^\circ$ [kJ kg <sup>-1</sup> ]		
$T_{ex}$ [K]		
$p_{C-J}$ [kbar]	228	
VoD [m s <sup>-1</sup> ]	7,389 (@ TMD)	
$V_0$ [L kg <sup>-1</sup> ]		

**Di(3,4-diamino-1,2,4-triazolium) 5-nitramino-tetrazolate**

Name [German, acronym]: Di(3,4-diamino-1,2,4-triazolium) 5-nitromino-tetrazolate  
[2DATr.NATZ]

Main (potential) use: Secondary explosive

Structural formula:



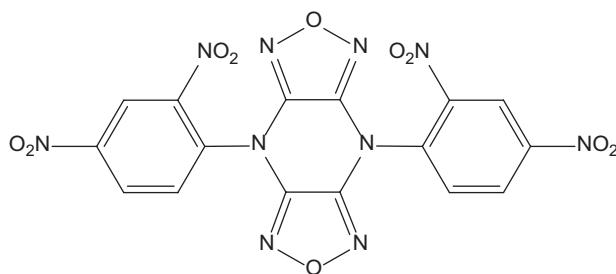
	2DATr.NATZ	
Formula	C <sub>5</sub> H <sub>12</sub> N <sub>16</sub> O <sub>2</sub> , [C <sub>2</sub> H <sub>6</sub> N <sub>5</sub> ] <sup>+</sup> <sub>2</sub> [CN <sub>6</sub> O <sub>2</sub> ] <sup>2-</sup>	
Molecular mass [g mol <sup>-1</sup> ]	328.13	
Appearance at RT		
IS [J]	25	
N [%]	68.27	
Ω(CO <sub>2</sub> ) [%]	-68.3	
T <sub>m.p.</sub> [°C]	157	
T <sub>dec.</sub> [°C]	227 (DSC @ 5 °C/min)	
ρ [g cm <sup>-3</sup> ]	1.674 (@ 153 K), 1.638 (@ 298 K)	
Heat of formation	386.1 kJ/mol (Δ <sub>f</sub> H <sup>o</sup> )	
	Calcd. (K-J)	Exptl.
-Δ <sub>ex</sub> U <sup>o</sup> [kJ kg <sup>-1</sup> ]		
T <sub>ex</sub> [K]		
p <sub>CJ</sub> [kbar]	253	
VoD [m s <sup>-1</sup> ]	7,717 (@ TMD)	
V <sub>0</sub> [L kg <sup>-1</sup> ]		

**4,8-Di(2,4-dinitrophenyl)difurazano[3,4-*b*:3',4'-*e*]pyrazine**

Name [German, acronym]: 4,8-di(2,4-Dinitrophenyl)difurazano[3,4-*b*:3',4'-*e*]pyrazine [4,8-di(2,4-dinitrophenyl)difurazano[3,4-*b*:3',4'-*e*]pyrazin]

Main (potential) use: Potential new heat-resistant explosive<sup>[1]</sup>

Structural formula:



	<b>4,8-di(2,4-dinitrophenyl)difurazano[3,4-<i>b</i>:3',4'-<i>e</i>]pyrazine</b>		
Formula	$C_{16}H_6N_{10}O_{10}$		
Molecular mass [g mol <sup>-1</sup> ]	498.28		
Appearance at RT	Red crystals <sup>[1]</sup>		
IS [J]	16 (ZBL-B instrument) <sup>[1]</sup>		
FS [N]	300 (FSKM 10 instrument) <sup>[1]</sup>		
ESD [J]	1.5 (ESD 2008A electric spark tester) <sup>[1]</sup>		
N [%]	28.11		
$\Omega(CO_2)$ [%]	-80.3		
$T_{dec.}$ [°C]	405 (DSC @ 10 °C/min) <sup>[1]</sup>		
$\rho$ [g cm <sup>-3</sup> ]	1.73 (crystal $\rho$ @ 293 K) <sup>[1]</sup> , 1.74 (gas pycnometer @ 25 °C) <sup>[1]</sup>		
Heat of formation	845.6 kJ/mol ( $\Delta H_f$ ) <sup>[1]</sup>		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{ex}U^\circ$ [kJ kg <sup>-1</sup> ]			
$T_{ex}$ [K]			

$p_{\text{C-J}}$ [kbar]		23.0 GPa (@ 1.74 g cm <sup>-3</sup> , $\Delta H_f = 845.6$ kJ/mol, calcd., K-J) <sup>[1]</sup>	
VoD [m s <sup>-1</sup> ]		7,200 (@ 1.74 g cm <sup>-3</sup> , $\Delta H_f = 845.6$ kJ/mol, calcd., K-J) <sup>[1]</sup>	
$V_0$ [L kg <sup>-1</sup> ]			

<b>4,8-di(2,4-dinitrophenyl)difurazano [3,4-<i>b</i>:3',4'-<i>e</i>]pyrazine<sup>[1]</sup></b>	
Chemical formula	C <sub>8</sub> H <sub>3</sub> N <sub>5</sub> O <sub>5</sub>
Molecular weight [g mol <sup>-1</sup> ]	249.15
Crystal system	Monoclinic
Space group	P2 <sub>1</sub> /n
<i>a</i> [\AA]	5.8796(12)
<i>b</i> [\AA]	8.9227(18)
<i>c</i> [\AA]	18.378(4)
$\alpha$ [°]	90
$\beta$ [°]	98.193
$\gamma$ [°]	90
<i>V</i> [\AA <sup>3</sup> ]	954.3(3)
<i>Z</i>	4
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.734
<i>T</i> [K]	296

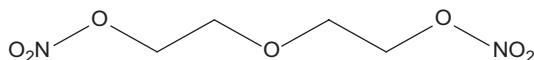
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## Diethyleneglycol dinitrate

Name [German, acronym]: Diethyleneglycol dinitrate, 2,2'-oxybisethanol dinitrate, dinitrodiglycol, diglycol dinitrate, dinitroethylene glycol, di-(ethyl-2-ol)ether dinitrate, 2,2'-dihydroxydiethylether dinitrate, nitrodiglycol (commercial) [diglykoldinitrat, dinitrodiglykol, DEGN, DEGDN, DNDG, DGDN]

Main (potential) use: Main component of double-base propellants<sup>[1]</sup>, in manufacture of flashless and non erosive low-calorific smokeless (double-base) powders<sup>[20]</sup>, plasticizer used in rocket propellants<sup>[33]</sup>, double-based smokeless propellants<sup>[33]</sup>, propellants<sup>[34]</sup>

Structural formula:



	<b>DEGN</b>
Formula	C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> O <sub>7</sub>
Molecular mass [g mol <sup>-1</sup> ]	196.12
Appearance at RT	Oily liquid <sup>[20]</sup> , exists in two crystalline forms: (i) stable form (melts @ 2 °C) and (ii) labile form (melts @ -10.9 °C) <sup>[20]</sup> , viscous, colorless, odorless liquid <sup>[22]</sup> , colorless <sup>[8,27]</sup> , clear, colorless, odorless liquid <sup>[18]</sup> , colorless liquid <sup>[29]</sup> , colorless, oily liquid <sup>[33]</sup> , colorless/pale oily liquid <sup>[34]</sup>
IS [J]	0.1 Nm <sup>[1]</sup> , 160 cm with 2 kg mass <sup>[12]</sup> , 175–180 cm (2 kg mass) <sup>[29]</sup> , 100 cm (2 kg mass, B.M.) <sup>[14]</sup> , 9 in (1 lb mass, P.A.) <sup>[14]</sup> , explodes if 2 kg mass dropped 160 cm <sup>[20]</sup> , H <sub>50</sub> = 160 cm <sup>[23]</sup> , 100+ cm (2 kg mass, 20 mg sample, B.M.) <sup>[8]</sup> , 9 in (2 kg mass, P.A.) <sup>[8]</sup> , 30 cm (median height, Rotter apparatus) <sup>[31]</sup> , H <sub>50</sub> = 2–3 cm (2 kg hammer, design no. 5 apparatus) <sup>[36]</sup> , H <sub>50</sub> = 98 cm (2.5 kg hammer, design no. 10 apparatus, liquid, tin foil covering) <sup>[36]</sup> , H <sub>50</sub> = 48.0 cm (2.5 kg hammer, design no. 13 apparatus) <sup>[36]</sup>

	Design no. 13 apparatus, liquids <sup>[36]</sup> :																								
	<table border="1"> <thead> <tr> <th>Drop height (cm)</th><th>Trials</th><th>% explosions</th></tr> </thead> <tbody> <tr><td>15</td><td>10</td><td>0</td></tr> <tr><td>20</td><td>20</td><td>5</td></tr> <tr><td>30</td><td>20</td><td>25</td></tr> <tr><td>40</td><td>20</td><td>20</td></tr> <tr><td>50</td><td>20</td><td>60</td></tr> <tr><td>60</td><td>20</td><td>75</td></tr> <tr><td>75</td><td>20</td><td>95</td></tr> </tbody> </table>	Drop height (cm)	Trials	% explosions	15	10	0	20	20	5	30	20	25	40	20	20	50	20	60	60	20	75	75	20	95
Drop height (cm)	Trials	% explosions																							
15	10	0																							
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60	20	75																							
75	20	95																							
FS [N]	Explodes with steel shoe (friction pendulum test) <sup>[8]</sup> , explodes in friction pendulum test <sup>[18]</sup>																								
N [%]	14.28																								
$\Omega(\text{CO}_2)$ [%]	-40.8																								
$T_{\text{m.p.}}$ [°C]	Stable modification: 2 <sup>[1,2,8,18]</sup> , unstable modification: -11.3 <sup>[1,3]</sup> , 2.0–3.6 (visual mpt., purified sample) <sup>[13]</sup> , 1.2–3.5 (visual mpt., as-received sample) <sup>[13]</sup> , 3.3 (endotherm onset, DSC @ 10 °C/min) <sup>[13]</sup> , -10.5 (labile crystals formed on rescanning melted sample, DSC @ 10 °C/min) <sup>[13]</sup> , -10.9 <sup>[23]</sup> , -11.8 <sup>[26]</sup> , 2 (stable form freezing point) <sup>[29]</sup> , -10.9 (labile form freezing point) <sup>[29]</sup> , -11.5 (freezing point) <sup>[22]</sup> , 2 <sup>[33]</sup> , 20 (stable form) <sup>[34]</sup> , -10.9 (unstable form) <sup>[34]</sup> , freezing point = -11.3 (or -12 °C) <sup>[34]</sup>																								
$T_{\text{b.p.}}$ [°C]	Boils with simultaneous dec. @ 160 °C <sup>[8,20]</sup> , 160–161 <sup>[18]</sup> , 160 <sup>[33,34]</sup>																								
$T_{\text{dec.}}$ [°C]	160 <sup>[34]</sup>																								
$T_{\text{glass transition}} (T_{g1/2})$ [°C]	No $T_g$ (DSC @ 10 °C/min) <sup>[13]</sup> , -86.9 (rerun, DSC @ 10 °C/min) <sup>[13]</sup> , -84 <sup>[24]</sup> , two crystalline forms: stable (mpt. = 20 °C) and unstable (mpt. = -10.9 °C) <sup>[34]</sup>																								
$\rho$ [g cm <sup>-3</sup> ]	1.3890 (@ 289.15 K) <sup>[4]</sup> , 1.385 (liq. @ 20 °C) <sup>[12,20]</sup> , 1.39 (@ 25 °C) <sup>[14]</sup> , 1.39 (@ TMD) <sup>[9]</sup> , 1.385 (@ 25 °C) <sup>[19]</sup> , $d^{16}_{16} = 1.3890^{[21]}$ , 1.38 <sup>[23,26,33]</sup> , 1.389 <sup>[25]</sup> , 1.38 (liquid) <sup>[8]</sup> , sp. gr. = 1.385 <sup>[18]</sup> , sp. gr. ( $z^\circ/15^\circ$ ) = 1.4092 (@ 0 °C) <sup>[22]</sup> , 1.3969 (@ 10 °C) <sup>[22]</sup> , 1.3846 (@ 20 °C) <sup>[22]</sup> , specific gravity $d^{20^\circ}_{15^\circ} = 1.385^{[29]}$ , $d^{16}_{16} = 1.3890^{[34]}$ , 1.385 <sup>[34]</sup>																								
Heat of formation	-437 kJ/mol ( $\Delta_f H^\ominus$ ) <sup>[5]</sup> , -416 kJ/mol ( $\Delta_f H^\ominus$ ) <sup>[9]</sup> , -2,227 kJ kg <sup>-1</sup> ( $\Delta_f H$ , ICT thermochemical database) <sup>[1,5]</sup> , -2,226 J/g ( $\Delta_f H$ ) <sup>[23]</sup> , -103.52 kcal/mol ( $\Delta_f H$ ) <sup>[14]</sup> , 526 kcal/kg ( $\Delta_f H^\ominus$ ) <sup>[16]</sup> , -426.8 kJ/mol (enthalpy of form.) <sup>[19]</sup> , -418.7 kJ/mol ( $\Delta_f H^\ominus$ ) <sup>[25]</sup> , 2,020 cal/g <sup>[8]</sup> , -99.4 kg cal/mol <sup>[18]</sup> , -437 kJ/mol (enthalpy of form.) <sup>[33]</sup> , 407.52 kJ/mol <sup>[34]</sup> , 428.02 kJ/mol (heat of form. under constant pressure) <sup>[34]</sup> , -99.4 kcal/mol ( $\Delta H_f^\ominus$ ) <sup>[35]</sup>																								
Heat of combustion	2,792 kcal/kg <sup>[8,16]</sup> , 2,297.4 kJ/mol <sup>[19]</sup> , $\Delta H_c = 11,707 \text{ J/g}$ <sup>[23]</sup> , 2,792 cal/g (@ C <sup>p</sup> ) <sup>[18]</sup> , 11,706.8 J/g (@ C <sup>V</sup> ) <sup>[34]</sup>																								

	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^{\circ}$ [kJ kg <sup>-1</sup> ]	4808	4,389 (calcd., K-J) <sup>[6]</sup> 3,240 (@ 1.38 g cm <sup>-3</sup> , calcd. BKWR) <sup>[10]</sup> 3,310 (@ 1.76 g cm <sup>-3</sup> , calcd. BKWR) <sup>[10]</sup> 3,690 (@ 1.38 g cm <sup>-3</sup> , calcd. BKWS) <sup>[10]</sup> 4,040 (@ 1.76 g cm <sup>-3</sup> , calcd. BKWS) <sup>[10]</sup> 841 kcal/kg <sup>[16]</sup> 4,566 J/g (calcd., ICT-code) <sup>[5]</sup> 4,565 J/g ( $\Delta H_{\text{e}}$ ) <sup>[23]</sup> 948 kcal/kg <sup>[29]</sup> 5.47 MJ/kg (calcd., SD method) <sup>[30]</sup> 4,140 [H <sub>2</sub> O (g)] <sup>[33]</sup>	4,566 [H <sub>2</sub> O (l)] <sup>[1,6]</sup> 4,141 [H <sub>2</sub> O (g)] <sup>[1]</sup> 841 cal/g <sup>[8]</sup> 4,476.0 J/g <sup>[12]</sup> 1,161 cal/g <sup>[18]</sup> 1,070 kcal/kg (on exploding @ 200 °C) <sup>[20]</sup>
$T_{\text{ex}}$ [K]	3338	3,083 (calcd., K-J) <sup>[5]</sup> 3,083 (calcd., ICT-code) <sup>[5]</sup> 3,485 (calcd., SD method) <sup>[30]</sup> 3,240 (@ 1.38 g cm <sup>-3</sup> , calcd. BKWR) <sup>[23]</sup> 3,690 (@ 1.38 g cm <sup>-3</sup> , calcd. BKWS) <sup>[23]</sup>	

$p_{CJ}$ [kbar]	181	132 (calcd., K-J) <sup>[5]</sup> 189 (@ 1.38 g cm <sup>-3</sup> , calcd. BKWR) <sup>[10]</sup> 266 (@ 1.76 g cm <sup>-3</sup> , calcd. BKWR) <sup>[10]</sup> 183 (@ 1.38 g cm <sup>-3</sup> , calcd. BKWS) <sup>[10]</sup> 239 (@ 1.76 g cm <sup>-3</sup> , calcd. BKWS) <sup>[10]</sup> 132.0 MPa (calcd., ICT-code) <sup>[5]</sup>	
VoD [m s <sup>-1</sup> ]	6,893 (@ 1.39 g cm <sup>-3</sup> , $\Delta_f H = -429.96$ kJ mol <sup>-1</sup> )	6,750 (@ 1.38 g cm <sup>-3</sup> (TMD), calcd. R-P method) <sup>[17]</sup> 7,080 (@ 1.38 g cm <sup>-3</sup> , calcd. BKWR) <sup>[10]</sup> 7,620 (@ 1.76 g cm <sup>-3</sup> , calcd. BKWR) <sup>[10]</sup> 7,190 (@ 1.38 g cm <sup>-3</sup> , calcd. BKWS) <sup>[10]</sup> 7,560 (@ 1.76 g cm <sup>-3</sup> , calcd. BKWS) <sup>[10]</sup> 6,600 (@ 1.38 g cm <sup>-3</sup> ) <sup>[33]</sup>	6,600 (@ 1.38 g cm <sup>-3</sup> ) <sup>[1]</sup> 6,760 (@ 1.38 g cm <sup>-3</sup> ) <sup>[7,8,9,10,14,18]</sup> 6,760 (@ 1.38 g cm <sup>-3</sup> ) <sup>[8]</sup> 6,800 (@ 1.38 g cm <sup>-3</sup> ) <sup>[15]</sup> DEGN detonates at either a high velocity of 6,800 m/s or a low velocity of 1,800–2,300 m/s <sup>[20]</sup> 6,922 ± 60 (@ 1.39 g cm <sup>-3</sup> , $D_i$ ) ( $D_i$ = ideal detonation velocity, steel tube) <sup>[30]</sup>
$V_0$ [L kg <sup>-1</sup> ]	847	919 <sup>[29]</sup>	991 <sup>[1,11]</sup> 796 <sup>[8]</sup>
$I_{sp}$ [NS g <sup>-1</sup> ]		2.42 (calcd., ISPBKW code) <sup>[35]</sup> , 2.47 (calcd., empirical) <sup>[35]</sup>	

Critical diameter [cm]	16 mm (high velocity detonation of DGDN) <sup>[25]</sup> , 16 mm <sup>[30]</sup>
Trauzl test [cm <sup>3</sup> , % TNT]	134–158% TNT <sup>[15]</sup> , 144–150% TNT <sup>[18]</sup> , 100% TNT <sup>[18]</sup> , 425 cm <sup>3</sup> (70% NG) <sup>[20]</sup> , 77% TNT <sup>[8]</sup> , 425 mL <sup>[29]</sup> , 410 <sup>[32]</sup>
Sand test [g]	95% TNT <sup>[15]</sup> , 42.2 g (200 g bomb) <sup>[8]</sup> , 100% TNT (modified sand test) <sup>[18]</sup>
Ballistic mortar test	127–135% TNT <sup>[15]</sup> , 90% TNT <sup>[8]</sup>

Ballistic pendulum test	127% TNT <sup>[18]</sup> , 90% NG <sup>[18]</sup>														
Gap test	Scale I (detonator = standard commercial no. 8 Briska type, donor = 2 × 20 g pellets of tetryl pressed to $\rho = 1.5$ 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 = 27 <sup>[28]</sup>														
5 s explosion $T$ [°C] 5 s ignition $T$ [°C] Explosion temperature test [°C]	237 <sup>[8]</sup> 237 (detonates) <sup>[27]</sup> 237 (USA value) <sup>[16]</sup> , 237 (Russian value) <sup>[16]</sup> 237 <sup>[18]</sup> , 200 <sup>[20]</sup>														
100 °C heat test [% mass loss]	4.0% mass loss in first 48 h <sup>[8]</sup> , 3.0% mass loss in second 48 h <sup>[8]</sup> , no explosion in 100 h <sup>[8]</sup>														
Abel heat test	>15 min <sup>[34]</sup>														
Thermal stability	Withstands long-term storage @ ordinary temperatures <sup>[18]</sup>														
Vacuum stability test [cm <sup>3</sup> /h]	0.33 cc/20 h/g @ 100 °C <sup>[8]</sup>														
Vapor pressure [atm @ °C]	0.0036 mm Hg @ 20 °C <sup>[8,18,20]</sup> , 0.130 mm Hg @ 60 °C <sup>[8,18,20]</sup> , 0.007 mm Hg @ 22.4 °C <sup>[22]</sup> , 0.00593 Torr @ 25 °C <sup>[18,26]</sup> , 0.0032 mm Hg @ 20 °C <sup>[34]</sup> , 0.130 mm Hg @ 60 °C <sup>[34]</sup>  Saturated vapor pressure (Pa) (statiscal and dynamic gas chromatography) <sup>[24]</sup> : 0.60 @ 25 °C, 0.92 @ 30 °C, 2.16 @ 40 °C, 4.26 @ 50 °C, 9.03 @ 60 °C <sup>[24]</sup>  0.0036 mm Hg @ 20 °C <sup>[29]</sup> , 0.130 mm Hg @ 60 °C <sup>[29]</sup>														
	<table border="1"> <thead> <tr> <th><math>T</math> (°C)</th> <th>Vapor pressure (mm Hg)<sup>[34]</sup></th> </tr> </thead> <tbody> <tr> <td>25</td> <td>0.0036</td> </tr> <tr> <td>60</td> <td>0.130</td> </tr> <tr> <td>70</td> <td>0.875</td> </tr> <tr> <td>80</td> <td>1.216</td> </tr> <tr> <td>90</td> <td>1.412</td> </tr> <tr> <td>100</td> <td>1.836</td> </tr> </tbody> </table>	$T$ (°C)	Vapor pressure (mm Hg) <sup>[34]</sup>	25	0.0036	60	0.130	70	0.875	80	1.216	90	1.412	100	1.836
$T$ (°C)	Vapor pressure (mm Hg) <sup>[34]</sup>														
25	0.0036														
60	0.130														
70	0.875														
80	1.216														
90	1.412														
100	1.836														
Volatility	193 mg/cm <sup>2</sup> /h @ 60 °C <sup>[8]</sup> , 0.19 mg/cm <sup>2</sup> /h @ 60 °C <sup>[18,20,34]</sup> , 193 mg/cm <sup>-2</sup> /h (@ 60 °C) <sup>[23]</sup> , 6.0% volatization @ 60 °C <sup>[34]</sup>														
Viscosity, $\eta$ [cP]	8.1 @ 20 °C <sup>[8,18,20,34]</sup> , 0.133 P @ 5.3 °C <sup>[21]</sup> , 0.0727 P @ 20.4 °C <sup>[21]</sup> , 0.0337 P @ 54.4 °C <sup>[21]</sup> , 8 @ 20 °C <sup>[29]</sup>  Viscosity values (no units given) from ref. <sup>[34]</sup> :														
	<table border="1"> <thead> <tr> <th><math>T</math> (°C)</th> <th>Viscosity, <math>\eta</math></th> </tr> </thead> <tbody> <tr> <td>6.0</td> <td>0.133</td> </tr> <tr> <td>20.4</td> <td>0.0727</td> </tr> <tr> <td>54.4</td> <td>0.0337</td> </tr> </tbody> </table>	$T$ (°C)	Viscosity, $\eta$	6.0	0.133	20.4	0.0727	54.4	0.0337						
$T$ (°C)	Viscosity, $\eta$														
6.0	0.133														
20.4	0.0727														
54.4	0.0337														

Burn rate [mm/s]	Not easy to burn cf. NG <sup>[34]</sup> , does not burn @ 15 °C in glass tube with 5–6 mm diameter <sup>[34]</sup> , burns @ 40 °C initial T or if diameter of glass tube is 8 mm <sup>[34]</sup> , linear rate of combustion is 50% that of nitrated ethylene glycol <sup>[34]</sup> , burn rate increases with increasing pressure <sup>[34]</sup>												
Solubility [g/mL]	<p>Readily soluble in Et<sub>2</sub>O, acetone, CHCl<sub>3</sub>, benzene, nitrobenzene, toluene, NG and glacial acetic acid<sup>[18]</sup>, insoluble in EtOH, CCl<sub>4</sub> and CS<sub>2</sub><sup>[18]</sup>, soluble in NG, nitroglycol, some common organic solvents<sup>[20]</sup>, 0.40 g/100 mL H<sub>2</sub>O @ 25 °C<sup>[8,18,20]</sup>, 0.46 g/100 mL H<sub>2</sub>O @ 60 °C<sup>[18,20]</sup>, 0.60 g/100 mL H<sub>2</sub>O @ 60 °C<sup>[8]</sup>, DEGDN dissolves NC<sup>[20]</sup>, completely miscible @ RT with NG, nitroglycol, Et<sub>2</sub>O, acetone, MeOH, CHCl<sub>3</sub>, benzene, glacial acetic acid<sup>[22]</sup>, soluble in H<sub>2</sub>O: 4.1 g dissolves in 1 L H<sub>2</sub>O @ 24 °C<sup>[22]</sup>, immiscible or only slightly soluble in EtOH, CCl<sub>4</sub>, CS<sub>2</sub><sup>[22]</sup>, aqueous solubility = 4,000 mg/L @ 25 °C<sup>[26]</sup>, insoluble in Et<sub>2</sub>O, EtOH, 2:1 Et<sub>2</sub>O:EtOH, acetone @ 25 °C<sup>[8]</sup>, readily soluble in NG, glycoldinitrate, Et<sub>2</sub>O and MeOH<sup>[29]</sup>, insoluble in EtOH, CCl<sub>4</sub> and CS<sub>2</sub><sup>[29]</sup>, 0.040 g dissolve in 100 g H<sub>2</sub>O @ 25 °C<sup>[29]</sup>, 0.46 g dissolve in 100 g H<sub>2</sub>O @ 60 °C<sup>[29]</sup>, soluble in NG, EGDN and other nitrates<sup>[34]</sup>, dissolves in Et<sub>2</sub>O, MeOH and other organic solvents<sup>[34]</sup>, low solubility in water<sup>[34]</sup>, 0.40 g/100 g H<sub>2</sub>O @ 25 °C<sup>[34]</sup>, 0.46 g/100 g H<sub>2</sub>O @ 60 °C<sup>[34]</sup>, 1.06% in 15% aq. nitric acid and increasing solubility as nitric acid concentration increases<sup>[34]</sup></p> <p>Aqueous solubility<sup>[34]</sup>:</p> <table border="1"> <thead> <tr> <th>T (°C)</th> <th>Solubility (%)</th> </tr> </thead> <tbody> <tr> <td>25</td> <td>0.4</td> </tr> <tr> <td>60</td> <td>0.46</td> </tr> <tr> <td>80</td> <td>0.63</td> </tr> <tr> <td>100</td> <td>0.92</td> </tr> <tr> <td>120</td> <td>1.37</td> </tr> </tbody> </table>	T (°C)	Solubility (%)	25	0.4	60	0.46	80	0.63	100	0.92	120	1.37
T (°C)	Solubility (%)												
25	0.4												
60	0.46												
80	0.63												
100	0.92												
120	1.37												
Hygroscopicity	Highly hygroscopic, must be stored in sealed containers <sup>[20]</sup> , slightly hygroscopic <sup>[22]</sup> , low hygroscopicity <sup>[34]</sup> , 0.19% @ 65% rel. humidity <sup>[34]</sup>												
Compatibility	Hydrolysis: 10 days @ 22 °C in 0.003% acid <sup>[8]</sup> , 5 days @ 60 °C in 0.003% acid <sup>[8]</sup> , readily plasticizes NC <sup>[29]</sup> , ready dec. with acids <sup>[34]</sup> , similar dec. in aqueous alkaline soln. as that of NG <sup>[34]</sup> , 0.003% acid value on hydrolysis in water after heating for 5 days @ 60 °C <sup>[34]</sup>												
Evaporation enthalpy [kJ/mol]	64.0 <sup>[24]</sup>												
Diffusion coefficient [cm <sup>2</sup> /s]	0.069 (air) <sup>[26]</sup> , 7.05 × 10 <sup>-6</sup> (water) <sup>[26]</sup>												
Log K <sub>ow</sub>	0.98 <sup>[26]</sup>												

Log $K_{oc}$	2.03 <sup>[26]</sup>
Biodegradation	Undergoes biodegradation <sup>[26]</sup>
Refractive index	$n_D^D = 1.4498^{[8]}$ , 1.450 @ 20 °C with Na light <sup>[18]</sup> , $n_D^{21.2} = 1.4505^{[34]}$ , 1.4517 @ 20 °C <sup>[34]</sup>
Flash point [°C]	210–215 <sup>[29]</sup>
Flame sensitivity	Insensitive to flame cf. NG <sup>[34]</sup> , difficult to ignite using direct flame <sup>[34]</sup>

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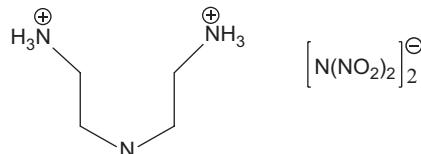
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## Diethylene-triamine bis-dinitramide

Name [German, acronym]: Diethylene-triamine bis-dinitramide, [diethylenetriamin bis-dinitramid, DETRA-D]

Main (potential) use: Possible TNT replacement<sup>[1]</sup>

Structural formula:



	DETRA-D		
Formula	$\text{C}_4\text{H}_{14}\text{N}_9\text{O}_8$		
Molecular mass [g mol <sup>-1</sup> ]	316.21		
Appearance at RT			
IS [J]	6.1 (50% prob., 2.5 kg, RT, 320 $\mu\text{m}$ sandpaper ( $\varnothing = 10$ mm) ERL type 12B, visual reaction and detected by microphone) <sup>[1]</sup>		
FS [N]	60 (average value from 10 trials, BAM Julius-Peters, porcelain plate and porcelain peg) <sup>[1]</sup>		
N [%]	39.87		
$\Omega(\text{CO}_2)$ [%]	-35.4		
$T_{\text{m.p.}}$ [ $^\circ\text{C}$ ]	79 <sup>[1]</sup>		
$T_{\text{dec.}}$ [ $^\circ\text{C}$ ]	160 (onset) <sup>[1]</sup>		
$\rho$ [g cm <sup>-3</sup> ]			
Heat of formation			
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^\ominus$ [kJ kg <sup>-1</sup> ]			
$T_{\text{ex}}$ [K]			
$p_{\text{C-J}}$ [kbar]			
VoD [m s <sup>-1</sup> ]			
$V_0$ [L kg <sup>-1</sup> ]			

Thermal stability	Thermometric TAM 2277 heat flow calorimeter, 19 days @ 75 °C: stable <sup>[1]</sup>																		
Compatibility	Block test, ocular inspection <sup>[1]</sup> : compatible with PETN, EPDM, stainless steel, Teflon, GUDN <sup>[1]</sup> ; incompatible with TNT, Fox-7, Al, RDX, Cu <sup>[1]</sup>  Thermometric TAM 2277 heat flow calorimeter, 19 days @ 75 °C: DETRA-D/teflon = compatible, DETRA-D/PETN = compatible, DETRA-D/GUDN = compatible, DETRA-D/EPDM = compatible, DETRA-D/stainless steel = compatible <sup>[1]</sup>																		
Castability	Melt-cast material and filler mixed in beaker heated @ 90 °C in water bath for several minutes, material filled into mold, inspected after 2 h <sup>[1]</sup> : <table border="1" style="margin-left: auto; margin-right: auto;"> <thead> <tr> <th>DETRA-D (wt.%)</th> <th>GUDN (wt.%)</th> <th>Result</th> </tr> </thead> <tbody> <tr> <td>100</td> <td>—</td> <td>Good cast</td> </tr> <tr> <td>70</td> <td>30</td> <td>Good cast</td> </tr> <tr> <td>50</td> <td>50</td> <td>Good cast</td> </tr> <tr> <td>40</td> <td>60</td> <td>Good cast</td> </tr> <tr> <td>30</td> <td>70</td> <td>Not castable</td> </tr> </tbody> </table>	DETRA-D (wt.%)	GUDN (wt.%)	Result	100	—	Good cast	70	30	Good cast	50	50	Good cast	40	60	Good cast	30	70	Not castable
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50	50	Good cast																	
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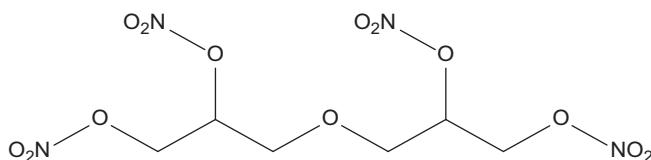
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## Diglycerol tetranitrate

Name [German, acronym]: Diglycerol tetranitrate, diglycerin tetranitrate, tetranitrodiglycerin [tetranitrodiglycerol, tetranitrodiglycerin, DGTN]

Main (potential) use: Manufacture of nonfreezing dynamites<sup>[1,3]</sup>, plasticizer in explosive and propellant and formulations<sup>[4]</sup>, similar properties to NG<sup>[4]</sup>

Structural formula:



	Diglycerol tetranitrate		
Formula	C <sub>6</sub> H <sub>10</sub> N <sub>4</sub> O <sub>13</sub>		
Molecular mass [g mol <sup>-1</sup> ]	346.16		
Appearance at RT	Very viscous oil <sup>[3]</sup> , not obtained in cryst. state <sup>[3]</sup> , clear colorless oil <sup>[4]</sup> , does not crystallize <sup>[4]</sup> , viscous oil <sup>[6]</sup>		
IS [J]	1.5 Nm <sup>[1]</sup> , 13 cm (2 kg mass, ~ 25 mg sample, 99 wt.% of DGTN/1 wt.% of 2-NDA) <sup>[4]</sup>		
FS [N]	75 lb @ 3 ft/s (99 wt.% of DGTN/ 1 wt.% of 2-NDA, ABL apparatus) <sup>[4]</sup>		
N [%]	16.19		
Ω(CO <sub>2</sub> ) [%]	-18.5		
T <sub>m.p.</sub> [°C]	*		
T <sub>dec.</sub> [°C]	178 (onset), 201 (peak max.) (DSC @ 5 °C/h, hermetic sealed Al pans, 99 wt.% DGTN, 1 wt.% 2-NDA) <sup>[4]</sup>		
ρ [g cm <sup>-3</sup> ]	1.52 <sup>[1]</sup> , 1.638 ± 0.06 (@ 293.15 K) <sup>[2]</sup>		
Heat of formation			
	Calcd. (K-J)	Lit. values	Exptl.
-Δ <sub>ex</sub> U <sup>o</sup> [kJ kg <sup>-1</sup> ]		1,370 kcal/kg <sup>[6]</sup>	

$T_{\text{ex}}$ [K]			
$p_{\text{C}_1}$ [GPa]			
VoD [ $\text{m s}^{-1}$ ]			
$V_0$ [ $\text{L kg}^{-1}$ ]			

\* Does not crystallize on cooling<sup>[6]</sup>

Trauzl test [ $\text{cm}^3$ , % TNT]	470 <sup>[5]</sup>
Vacuum stability test [ $\text{cm}^3/\text{h}$ ]	0.342 mL/g (1 g sample, 40 h @ 90 °C, 99 wt.% DGTN, 1 wt.% 2-NPDA) <sup>[4]</sup>
Solubility [g/mL]	Insoluble in $\text{H}_2\text{O}$ <sup>[3,4,6]</sup> , readily soluble in EtOH and $\text{Et}_2\text{O}$ <sup>[3]</sup> , insoluble in common organic solvents <sup>[4]</sup> , soluble in $\text{CH}_2\text{Cl}_2$ <sup>[4]</sup> , readily soluble in EtOH, $\text{Et}_2\text{O}$ and other common organic solvents <sup>[6]</sup>
Hygroscopicity	Nonhygroscopic <sup>[3,4,6]</sup>
SBAT [°C]	118 (onset, burned) (simulated bulk autoignition test, ramp rate = 4.4 °C/h, 99 wt.% of DGTN, 1 wt.% of 2-NPDA) <sup>[4]</sup>
Decomposition energy [J/g]	~4,500–4,700 <sup>[4]</sup>
Viscosity	11 × that of glycerol <sup>[6]</sup>

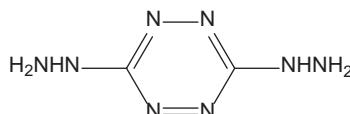
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## 1,4-Dihydrazino tetrazine

Name [German, acronym]: 3,6-Dihydrazine-1,2,4,5-tetrazine, dihydrazinyl-1,2,4,5-tetrazine [1,4-dihydrazino tetrazin, DHTz, DHT]

Main (potential) use: Possible applications in future pyrotechnic formulations<sup>[1]</sup>, possible future application in rocket and gun propellants<sup>[3]</sup>

Structural formula:



	DHTz		
Formula	C <sub>2</sub> H <sub>6</sub> N <sub>8</sub>		
Molecular mass [g mol <sup>-1</sup> ]	142.13		
Appearance at RT			
IS [J]	H <sub>50</sub> = 70 cm <sup>[2]</sup> , H <sub>50</sub> = 65 cm <sup>[3,4]</sup>		
FS [N]	8% <sup>[2]</sup> , >36 kg <sup>[4]</sup>		
ESD [J]	0 goes out of 13 @ 0.36 J <sup>[4]</sup>		
N [%]	78.84		
Ω(CO <sub>2</sub> ) [%]	-78.8		
T <sub>m.p.</sub> [°C]	No mpt. <sup>[3]</sup>		
T <sub>b.p.</sub> [°C]	425 (est.) <sup>[3]</sup>		
T <sub>dec.</sub> [°C]	162.9 (exo peak max, DSC @ 10 °C/min) <sup>[2]</sup> , 156 (exo peak max, DSC @ 4 °C/min) <sup>[3]</sup> , 167 (exo peak max, DSC @ 8 °C/min) <sup>[3]</sup> , 173 (exo peak max, DSC @ 16 °C/min) <sup>[3]</sup> , 182 (exo peak max, DSC @ 32 °C/min) <sup>[3]</sup> , 193 (exo peak max, DSC @ 64 °C/min) <sup>[3]</sup> , 160 (onset, DSC) <sup>[4]</sup>		
ρ [g cm <sup>-3</sup> ]	1.69 <sup>[2,3]</sup> , 1.59 (pressed strand) <sup>[3]</sup>		
Heat of formation	535.0 kJ/mol (ΔH <sub>f</sub> ) <sup>[2]</sup> , 536 kJ/mol (measured) <sup>[3]</sup> , 535.55 kJ/mol (Δ <sub>f</sub> H <sup>o</sup> ) <sup>[3]</sup>		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
-Δ <sub>ex</sub> U <sup>o</sup> [kJ kg <sup>-1</sup> ]			

$T_{\text{ex}}$ [K]																																											
$p_{\text{CJ}}$ [kbar]																																											
VoD [ $\text{m s}^{-1}$ ]		9,234 (@ $1.69 \text{ g cm}^{-3}$ ) <sup>[2]</sup>	7,540 (@ $1.56 \text{ g cm}^{-3}$ , unconfined pellets of 1.25 cm diameter) <sup>[3]</sup>																																								
$V_0$ [ $\text{L kg}^{-1}$ ]																																											
Thermal stability	Volume of dec. gases ( $\text{cm}^3/\text{g}$ ) released over time @ various $T$ , approx. values <sup>[3]</sup> :																																										
	<table border="1" style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th colspan="4" style="text-align: center;"><math>T</math> (°C)</th></tr> <tr> <th style="text-align: center;">110</th><th style="text-align: center;">115</th><th style="text-align: center;">120</th><th style="text-align: center;">130</th></tr> </thead> <tbody> <tr> <td style="text-align: center;">5 (25 min)</td><td style="text-align: center;">10 (25 min)</td><td style="text-align: center;">20 (25 min)</td><td style="text-align: center;">25 (20 min)</td></tr> <tr> <td style="text-align: center;">5.5 (50 min)</td><td style="text-align: center;">20 (70 min)</td><td style="text-align: center;">20 (50 min)</td><td style="text-align: center;">125 (40 min)</td></tr> <tr> <td style="text-align: center;">10 (90 min)</td><td style="text-align: center;">30 (110 min)</td><td style="text-align: center;">55 (80 min)</td><td style="text-align: center;">190 (45 min)</td></tr> <tr> <td style="text-align: center;">25 (30 min)</td><td style="text-align: center;">35 (140 min)</td><td style="text-align: center;">105 (90 min)</td><td style="text-align: center;">200 (50 min)</td></tr> <tr> <td style="text-align: center;">30 (60 min)</td><td style="text-align: center;">45 (150 min)</td><td style="text-align: center;">130 (110 min)</td><td style="text-align: center;">210 (80 min)</td></tr> <tr> <td style="text-align: center;">30 (200 min)</td><td style="text-align: center;">80 (170 min)</td><td></td><td></td></tr> <tr> <td style="text-align: center;">60 (270 min)</td><td style="text-align: center;">125 (180 min)</td><td></td><td></td></tr> <tr> <td style="text-align: center;">80 (300 min)</td><td></td><td></td><td></td></tr> </tbody> </table>			$T$ (°C)				110	115	120	130	5 (25 min)	10 (25 min)	20 (25 min)	25 (20 min)	5.5 (50 min)	20 (70 min)	20 (50 min)	125 (40 min)	10 (90 min)	30 (110 min)	55 (80 min)	190 (45 min)	25 (30 min)	35 (140 min)	105 (90 min)	200 (50 min)	30 (60 min)	45 (150 min)	130 (110 min)	210 (80 min)	30 (200 min)	80 (170 min)			60 (270 min)	125 (180 min)			80 (300 min)			
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Vacuum stability test [ $\text{cm}^3/\text{h}$ ]	15.83 mL/g @ 100 °C <sup>[4]</sup>																																										
Burn rate [mm/s]	Burns with little or no luminous flame <sup>[3]</sup>																																										
Flame $T$ [K]	1,180 °C (max) <sup>[3]</sup>																																										
Average surface $T$ [°C]	$261 \pm 10$ @ 0.2 atm <sup>[3]</sup> , $395 \pm 11$ @ 0.5 atm <sup>[3]</sup>																																										
Heat of vaporization [kJ/mol]	95.0 (est.) <sup>[3]</sup>																																										
Thermal diffusivity [ $\text{cm}^2\text{s}^{-1}$ ]	$(2.0 \pm 0.3) \times 10^{-3}$ (molten DHT @ $T < 700$ K) <sup>[3]</sup>																																										
Laser ignition	Ignition delay (s) as a function of laser irradiance ( $\text{W/cm}^2$ ) (approx. values from graph): 0.7 s/20 W/cm <sup>2</sup> , 0.4 s/30 W/cm <sup>2</sup> , 0.25 s/35 W/cm <sup>2</sup> , 0.15 s/45 W/cm <sup>2</sup> , 0.12 s/65 W/cm <sup>2</sup> , 0.65 s/85 W/cm <sup>2</sup> <sup>[4]</sup>																																										

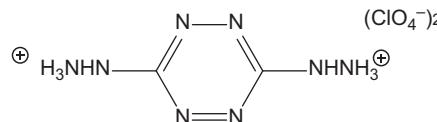
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- [3] V. P. Sinditskii, V. Y. Egorshev, G. F. Rudakov, A. V. Burzhava, S. A. Filatov, L. D. Sang, *Thermochim. Acta*, 2012, 535, 48–57.
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## 3,6-Dihydrazino-1,2,4,5-tetrazine diperchlorate salt

Name [German, acronym]: Diperchlorate salt of 3,6-dihydrazino-1,2,4,5-tetrazine,  
[3,6-dihydrazino-1,2,4,5-tetrazin diperchlorat Salz]

Main (potential) use:

Structural formula:



	3,6-Dihydrazino-1,2,4,5-tetrazine diperchlorate salt		
Formula	C <sub>2</sub> H <sub>8</sub> Cl <sub>2</sub> N <sub>8</sub> O <sub>8</sub>		
Molecular mass [g mol <sup>-1</sup> ]	343.03		
Appearance at RT			
IS [J]	13 cm <sup>[1]</sup> , H <sub>50</sub> = 8.7 cm <sup>[2]</sup>		
N [%]	32.67		
Ω(CO <sub>2</sub> ) [%]			
T <sub>dec.</sub> [°C]	200 (exo, DTA) <sup>[1]</sup> , 197.4 (DSC @ 10 °C/min) <sup>[2]</sup>		
ρ [g cm <sup>-3</sup> ]	1.96 (flotation) <sup>[1]</sup> , 1.77 <sup>[2]</sup>		
Heat of formation	-69.3 kJ/mol (ΔH <sub>f</sub> ) <sup>[2]</sup>		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
-Δ <sub>ex</sub> U <sup>o</sup> [kJ kg <sup>-1</sup> ]			
T <sub>ex</sub> [K]			
p <sub>C,I</sub> [kbar]			
VoD [m s <sup>-1</sup> ]			
V <sub>0</sub> [L kg <sup>-1</sup> ]			

[1] D. E. Chavez, M. A. Hiskey, *J. Energet. Mater.*, **1999**, *17*, 357–377.

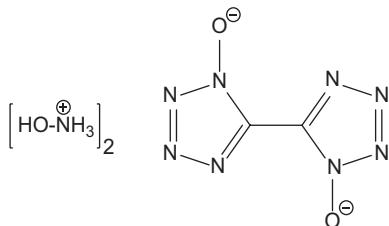
[2] H.-H. Zhang, S.-Y. Jia, B.-Z. Wang, X.-J. Wang, C. Zhou, W.-P. Lai, J.-Z. Li, *Chinese J. Explosives, Propellants*, **2014**, *37*, 23–30.

## Dihydroxylammonium 5,5'-bitetrazole-1,1'-dioxide

Name [German, Acronym]: Dihydroxylammonium 5,5'-bitetrazole-1,1'-dioxide  
 [dihydroxylammonium 5,5'-bitetrazol-1,1'-dioxid,  
 TKX-50, HATO]

Main (potential) use: Secondary (high) explosive

Structural formula:



	TKX-50
Formula	$\text{C}_2\text{H}_8\text{N}_{10}\text{O}_4$ , $[\text{H}_4\text{NO}]^{+2} [\text{C}_2\text{N}_8\text{O}_2]^{2-}$
Molecular mass [g mol <sup>-1</sup> ]	236.2
Appearance at RT	Colorless crystals
IS [J]	20 (1/6, BAM) <sup>[1,13]</sup> , 56 <sup>[10]</sup> , 50 (after 2 h ball milling) <sup>[10]</sup> , 71.25 cm (calcd. empirical method, 2.5 kg mass) <sup>[16]</sup> , $H_{50} = 103.3$ cm (2 kg hammer, WL-1 apparatus, nano-TKX-50) <sup>[17]</sup> , $H_{50} \geq 120$ cm (2 kg hammer, WL-1 apparatus, millisized TKX-50) <sup>[17]</sup>
FS [N]	120 (1/6, BAM) <sup>[1,13]</sup> , 50 <sup>[10]</sup> , 40 (after 2 h ball milling) <sup>[10]</sup> , 75% probability of explosion (nano-TKX-50, MGY-1-type friction apparatus, 2 kg pendulum hammer, <90° tilt angle, 3.0 MPa pressure, 20 mg sample) <sup>[17]</sup> , 85% probability of explosion (millisized TKX-50, MGY-1-type friction apparatus, 2 kg pendulum hammer, <90° tilt angle, 3.0 MPa pressure, 20 mg sample) <sup>[17]</sup>
ESD [J]	0.1 <sup>[1]</sup>
N [%]	59.3
$\Omega(\text{CO}_2)$ [%]	-27.1
$T_{\text{m.p.}}$ [°C]	Exothermic dec. without prior melting at 247.8 (DSC) <sup>[18]</sup>

$T_{\text{dec.}} [^{\circ}\text{C}]$	221 (DSC @ 5 °C/min) <sup>[1]</sup> , 221 <sup>[13]</sup> , 511 K (onset), 516 K (exo, peak max), 546 K (exo, second peak max) (DSC @ 10 K/min) <sup>[15]</sup> , 510 K (55% mass loss, TG, 1 mg sample @ 10 K/min) <sup>[15]</sup> , 443–463 K (average total mass loss = 49%, Ar flow (0.1 MPa)) <sup>[15]</sup> , 251 (exo, peak 1), 308 (exo peak 2) (DSC @ 10 °C/min) <sup>[19]</sup> , 242 (exo, peak 1), 302 (exo peak 2) (DSC @ 5 °C/min) <sup>[19]</sup> , 231 (exo, peak 1), 291 (exo peak 2) (DSC @ 2 °C/min) <sup>[19]</sup> , 226 (exo, peak 1), 287 (exo peak 2) (DSC @ 1 °C/min) <sup>[19]</sup> , 247.8 (exo, DSC) <sup>[18]</sup> , 13.58% mass loss (@ 130–195, first stage dec., TG @ 10 °C/min), 73.50% mass loss (@ 195–330 °C, second stage dec., TG @ 10 °C/min) <sup>[18]</sup> , 66.10% mass loss (@ 225.10–247.83 °C, first stage mass loss, peak max. in DTG @ 235.50 °C, @ 10 °C/min), 26.97% mass loss (@ 247.83–272.66 °C), second stage mass loss, peak max in DTG @ 256.33 °C, @ 10 °C/min <sup>[20]</sup> , 200.2 (first stage dec. onset, ARC) <sup>[21]</sup> , 250.6 (exo peak 1 max), 274.3 (exo peak 2 max) (DSC @ 10 °C/min, millisized particles) <sup>[17]</sup> , 236.0 (exo peak 1 max), 259.7 (exo peak 2 max) (DSC @ 10 °C/min, nanosized particles) <sup>[17]</sup>																
$\rho [\text{g cm}^{-3}]$	1.918 (crystal @ 100 K) <sup>[1]</sup> , 1.877 (crystal) <sup>[9]</sup> , 1.915 (crystal @ 170 K) <sup>[1]</sup>  Relationship between $\rho$ and specific pressure <sup>[10]</sup> :																
	<table border="1"> <thead> <tr> <th><math>\rho (\text{g cm}^{-3})</math></th><th>Specific pressure</th></tr> </thead> <tbody> <tr><td>1.63</td><td>1,000</td></tr> <tr><td>1.68</td><td>1,500</td></tr> <tr><td>1.715</td><td>2,000</td></tr> <tr><td>1.735</td><td>2,500</td></tr> <tr><td>1.75</td><td>3,000</td></tr> <tr><td>1.76</td><td>3,500</td></tr> </tbody> </table>			$\rho (\text{g cm}^{-3})$	Specific pressure	1.63	1,000	1.68	1,500	1.715	2,000	1.735	2,500	1.75	3,000	1.76	3,500
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1.735	2,500																
1.75	3,000																
1.76	3,500																
Heat of formation	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.														
$-\Delta_{\text{ex}} U^{\circ} [\text{kJ kg}^{-1}]$	5,984	6,025 <sup>[7]</sup>	4,650 J/g (TKX-50-based molding particles) <sup>[10]</sup>														
$T_{\text{ex}} [\text{K}]$	3,620	3,954 <sup>[9]</sup>  2,433 (@ 1.877 g cm <sup>-3</sup> , $\Delta H_f = 193 \text{ kJ/mol}$ , calcd., JAGUAR) <sup>[11]</sup>  3,724 (calcd., empirical) <sup>[9]</sup>															

$p_{C_J}$ [kbar]	408	424 <sup>[7,9]</sup>  42.1 GPa (@ 1.877 g cm <sup>-3</sup> , $\Delta H_f = 193$ kJ/mol, calcd., JAGUAR) <sup>[11]</sup>  418.95 (calcd., empirical) <sup>[9]</sup>															
VoD [m s <sup>-1</sup> ]	10,027 (@ TMD)	9,698 ( $\rho$ not specified) <sup>[7]</sup>  9,735 (@ TMD, 1.877 g cm <sup>-3</sup> , calcd., CHEETAH v8.0) <sup>[8]</sup>  9,190 (@ $\rho$ not specified) <sup>[9]</sup>  9,830 (@ 1.877 g cm <sup>-3</sup> , $\Delta H_f = 193$ kJ/mol, calcd., JAGUAR) <sup>[11]</sup>  9,650 (@ 1.877 g cm <sup>-3</sup> , calcd., empirical) <sup>[9]</sup>	9,432 (@ TMD, large-scale detonation test) <sup>[8]</sup>  9,560 (est., LASEM method) <sup>[8]</sup>  8,950 (@ 1.74 g cm <sup>-3</sup> )  VoD of TKX-based explosives with different $\rho$ , TKX-50/binder, 95.5/4.5, TKX-50 (95.5%), ETPE (3%), graphite and other materials (1.5%), values determined using Cu probe method <sup>[11]</sup> :														
			<table border="1"> <thead> <tr> <th><math>\rho</math> (g cm<sup>-3</sup>)</th> <th>VoD (m/s)</th> </tr> </thead> <tbody> <tr> <td>1.555</td> <td>7,976</td> </tr> <tr> <td>1.606</td> <td>8,248</td> </tr> <tr> <td>1.658</td> <td>8,472</td> </tr> <tr> <td>1.697</td> <td>8,716</td> </tr> <tr> <td>1.702</td> <td>—</td> </tr> <tr> <td>1.740</td> <td>8,904</td> </tr> </tbody> </table>	$\rho$ (g cm <sup>-3</sup> )	VoD (m/s)	1.555	7,976	1.606	8,248	1.658	8,472	1.697	8,716	1.702	—	1.740	8,904
$\rho$ (g cm <sup>-3</sup> )	VoD (m/s)																
1.555	7,976																
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1.697	8,716																
1.702	—																
1.740	8,904																
			<i>See additional values later</i>														
$V_0$ [L kg <sup>-1</sup> ]	923																
$I_{sp}$ [Ns g <sup>-1</sup> ]	2.65 (calcd., ISPBKW code) <sup>[12]</sup> , 2.63 (calcd., empirical) <sup>[12]</sup> , 261 s (assuming isobaric 60 bar conditions, calcd., EXPLO5.05) <sup>[1]</sup> , 2.56 (calcd., empirical) <sup>[9]</sup>																

Detonation velocities of TKX-based explosives with different diameters, TKX-50 (95.5%), ETPE (3%), graphite and other materials (1.5%), sample prepared under specific pressure of 3,000, values determined using Cu probe method<sup>[11]</sup>:

Sample	Standards (mm)	$\rho$ (g cm <sup>-3</sup> )	Detonation velocity (ms <sup>-1</sup> )
TKX-50/binder 95.5/4.5	Φ 20 mm × 20 mm	1.79	8,699
	Φ 30 mm × 30 mm	1.80	8,774
	Φ 40 mm × 40 mm	1.80	8,994
	Φ 50 mm × 50 mm	1.81	8,996
	Φ 60 mm × 60 mm	1.80	9,037

Critical diameter [cm]	Steady detonation perhaps only possible when column diameters $\geq$ 30 mm <sup>[10]</sup>
Trauzl test [cm <sup>3</sup> , % TNT]	140% TNT (calcd., empirical) <sup>[9]</sup>
Gap test	Thickness of the organic glass gap and the correspondingly pressure of shock wave values of TKX-based explosive (TKX-50 (95.5%), ETPE (3%), graphite and other materials (1.5%)), sample prepared under specific pressure of 3,000 <sup>[10]</sup> : thickness = 18.45 mm, pressure = 6.24 GPa <sup>[10]</sup>
Thermal stability	$T_0$ (onset self-heating temperature) = 454 K (ARC) <sup>[15]</sup> , 129.01 °C (SAD simulation of 25 kg of TKX-50 packaged in polyethylene can) <sup>[20]</sup> , TMRad = 142.12 °C (calcd.) <sup>[20]</sup> , unaffected by heating @ 75 °C for 48 h (open glass vessel, DSC) <sup>[1]</sup> , $T_{NR}$ = 195.14 °C, SADT = 191.52 °C (nano-TKX-50) <sup>[24]</sup> , $T_{NR}$ = 188.69 °C, SADT = 182.53 °C (micro-TKX-50) <sup>[24]</sup> , $T_{NR}$ = 208.73 °C, SADT = 205.31 °C (milli-TKX-50) <sup>[24]</sup> , good thermal stability during storage and transportation process <sup>[24]</sup>
Compatibility	Stable for 14 days @ 25 °C or for 48 h @ 50 °C in DMSO, deionized water, ethyl acetate, acetonitrile, MeOH, EtOH, petroleum ether, hexane <sup>[14]</sup> , unstable in DMF @ 25 °C and 50 °C <sup>[14]</sup> , unstable in DMF/acetone@ 25 °C and in DMF/DMSO @ 25 °C <sup>[14]</sup> , compatibility rating A-D based on DSC measurements: DNAN = A-B, TNT = C, RDX = D, HMX = B, CL-20 = C, centralite = C, NC = C, NC + NG = D AP = C, HNE = A, Al = C, boron = D, GAP = C, HTPB = D <sup>[25]</sup> , good compatibility with TNT in TKX-50/TNT mass ratios 50:50, 40:60, 30:70, 20:80, 10:90 <sup>[19]</sup>
$\Delta H_{fusion}$ [kJ/mol]	38.45 (calcd.) <sup>[9]</sup> , 38.5 <sup>[9]</sup>

Chemical affinity	Chemical affinities between TKX-50 and different binders <sup>[10]</sup> :				
		(0 0 1)	(0 1 0)	(1 0 0)	Average values
	TKX-50/F26	100.01	41.85	33.14	58.33
	TKX-50/EVA	28.34	60.41	47.40	45.38
	TKX-50/EPDM	18.70	23.83	34.83	25.79
TKX-50/ETPE	113.52	132.94	86.84	111.10	
Heat of dec. [J/g]	$2,320 \pm 190$ (average value, Al pans covered with pierced lids) <sup>[15]</sup>				
Koenen test	10 mm orifice, 23.0 g TKX-50, ruptures into approx. 100 pieces <sup>[1]</sup>				
Fast cook-off test	No explosion observed, only controlled deflagration <sup>[1]</sup>				
Heat capacity [kJ/mol]	295 (@ constant pressure @ RT) <sup>[26]</sup> , 292 (@ constant volume @ RT) <sup>[26]</sup>				

	TKX-50 <sup>[1]</sup>	TKX-50 <sup>[1]</sup>	TKX-50 <sup>[1]</sup>	TKX-50 <sup>[27]</sup>
Chemical formula	C <sub>2</sub> H <sub>8</sub> N <sub>10</sub> O <sub>4</sub>	C <sub>2</sub> H <sub>8</sub> N <sub>10</sub> O <sub>4</sub>	C <sub>2</sub> H <sub>8</sub> N <sub>10</sub> O <sub>4</sub>	C <sub>2</sub> H <sub>8</sub> N <sub>10</sub> O <sub>4</sub>
Molecular weight [g mol <sup>-1</sup> ]	236.18	236.18	236.18	236.18
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	P <sub>2</sub> <sub>1</sub> /c (no. 14)			
<i>a</i> [Å]	5.4408(6)	5.4260(5)	5.4872(8)	5.49040(10)
<i>b</i> [Å]	11.7514(13)	11.6597(12)	11.5472(15)	11.4912(3)
<i>c</i> [Å]	6.5612(9)	6.5013(7)	6.4833(9)	6.45560(10)
$\alpha$ [°]	90	90	90	90
$\beta$ [°]	95.071(11)	95.256(9)	95.402(12)	95.5710(16)
$\gamma$ [°]	90	90	90	90
<i>V</i> [Å <sup>3</sup> ]	417.86(9)	409.58(7)	408.97(10)	405.368(14)
<i>Z</i>	2	2	2	2
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.877	1.915	1.918	1.935
<i>T</i> [K]	298	173	100	20

In the anisotropic thermal expansion, negative thermal expansion along the *a*-axis of the unit cell was observed and in addition, the  $\beta$ -angle was also observed to decrease ( $-0.27\%$  from 30 °C to 175 °C). In contrast, the *b*-axis increased by 0.96%, the *c*-axis by 0.50% and the unit cell volume, *V*, by 1.42%, which corresponded to positive thermal expansion<sup>[28]</sup>.

The calculated pressure-induced changes in the unit cell parameters of TKX-50 show that the compressibility of the TKX-50 single crystal to be highly anisotropic with extremely low compressibility along the *a*-axis ( $a/a_0 = 97\%$ ,  $b/b_0 = 83\%$ ,  $c/c_0 = 88\%$ )<sup>[29]</sup>.

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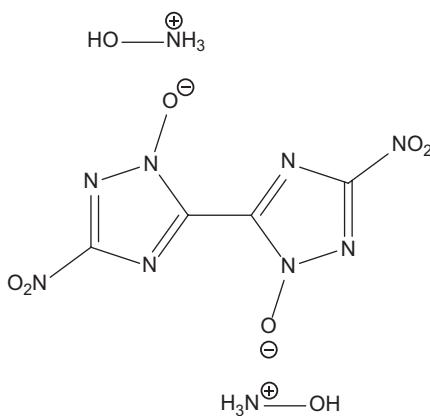
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## Dihydroxylammonium-3,3'-dinitro-5,5'-bis(1,2,4-triazole)-1,1'-diolate

Name [German, acronym]: Dihydroxylammonium-3,3'-dinitro-5,5'-bis(1,2,4-triazole)-1,1'-diolate, [dihydroxylammonium-3,3'-dinitro-5,5'-bis(1,2,4-triazole)-1,1'-diolate, MAD-X1, Hx2-DNBTO]

Main (potential) use: High explosive<sup>[1]</sup>

Structural formula:



	<b>MAD-X1</b>
Formula	C <sub>4</sub> H <sub>8</sub> N <sub>10</sub> O <sub>8</sub>
Molecular mass [g mol <sup>-1</sup> ]	324.17
Appearance at RT	Orange block crystals <sup>[2]</sup>
IS [J]	>40 <sup>[2,6]</sup>
FS [N]	>360 <sup>[2,6]</sup>
ESD [J]	0.5 <sup>[2]</sup>
N [%]	43.21
Ω(CO <sub>2</sub> ) [%]	-19.74
T <sub>m.p.</sub> [°C]	No mpt. observed in DSC @ 5 °C/min <sup>[6]</sup>
T <sub>dec.</sub> [°C]	217 (DSC @ 5 °C/min) <sup>[2]</sup> , 248.7 (DSC @ 5 °C/min) <sup>[6]</sup> , two stage dec. process: 213.41 (stage 1 mass loss), 242.58 (stage 2 mass loss), total of 86.88% dec. @ 265 °C (TG-DTG) <sup>[6]</sup>
ρ [g cm <sup>-3</sup> ]	1.90 (@ 298.15 K) <sup>[2]</sup>

Heat of formation	213 kJ/mol ( $\Delta_f H^\circ$ ) <sup>[2]</sup> , 657 kJ kg <sup>-1</sup> ( $\Delta_f H^\circ$ ) <sup>[2]</sup>		
	Calcd. (EXPLO5)	Lit. values	Exptl.
$-\Delta_{\text{ex}} U^\circ$ [kJ kg <sup>-1</sup> ]	5,985 <sup>[2]</sup>		
T <sub>ex</sub> [K]	4,153 <sup>[2]</sup>	2,897 (@ 1.90 g cm <sup>-3</sup> , $\Delta H_f = -149.4$ kJ/mol, calcd., JAGUAR) <sup>[5]</sup>	
p <sub>C-J</sub> [kbar]	133 <sup>[3]</sup>	36.5 GPa (@ 1.90 g cm <sup>-3</sup> , $\Delta H_f = -149.4$ kJ/mol, calcd., JAGUAR) <sup>[5]</sup>	336 <sup>[1]</sup>
VoD [m s <sup>-1</sup> ]	9,195 (@ TMD) <sup>[4]</sup>	8,950 (@ 1.90 g cm <sup>-3</sup> , $\Delta H_f = -149.4$ kJ/mol, calcd., JAGUAR) <sup>[5]</sup>  9,267 (@ TMD, calcd., CHEETAH v8.0) <sup>[4]</sup>	8,860 ± 220 (@ TMD) <sup>[4]</sup>  8,853 (@ 1.8 g cm <sup>-3</sup> ) <sup>[1]</sup>
V <sub>0</sub> [L kg <sup>-1</sup> ]	734 <sup>[2]</sup>		

	MAD-X1 <sup>[2]</sup>
Chemical formula	C <sub>4</sub> H <sub>8</sub> N <sub>10</sub> O <sub>8</sub>
Molecular weight [g mol <sup>-1</sup> ]	324.169
Crystal system	Monoclinic
Space group	P2 <sub>1</sub> /c (no. 14)
a [Å]	7.3072(9)
b [Å]	5.2430(8)
c [Å]	14.403(2)
α [°]	90
β [°]	91.498(13)
γ [°]	90
V [Å <sup>3</sup> ]	551.61(3)
Z	2
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.9518
T [K]	173

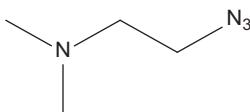
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## 2-Dimethylaminoethylazide

Name [German, acronym]: 2-(Dimethylamino)ethylazide, 2-azido-*N*, *N*-dimethyllethanamine [2-dimethylaminoethylazid, DMAZ, CINCH (competitive impulse noncarcinogenic hypergol)]

Main (potential) use: Possible replacement for the bipropellant fuels monomethyl hydrazine and dimethyl hydrazine<sup>[1]</sup>, possible monopropellant<sup>[4]</sup>, highly energetic liquid fuel<sup>[5]</sup>, possible replacement for hydrazine in space industries<sup>[6]</sup>

Structural formula:



	DMAZ
Formula	C <sub>4</sub> H <sub>10</sub> N <sub>4</sub>
Molecular mass [g mol <sup>-1</sup> ]	114.15
Appearance at RT	Achromatic color transparent light yellow liquid <sup>[3]</sup> , liquid <sup>[4]</sup> , colorless liquid <sup>[6]</sup>
IS [J]	165 kg cm <sup>-1</sup> <sup>[3]</sup> , negative @ 165 kg cm <sup>[4]</sup> , >98 (no response in 6 tests @ 1 m, 10 kg mass, BAM) <sup>[5]</sup>
FS [N]	500 psi <sup>[3]</sup> , negative @ 500 psi <sup>[4]</sup>
ESD [J]	<525 mJ <sup>[3,5]</sup>
N [%]	49.08
Ω(CO <sub>2</sub> ) [%]	-182.2
T <sub>m.p.</sub> [°C]	-68.9 (freezing point) <sup>[3,4]</sup>
T <sub>b.p.</sub> [°C]	135 <sup>[4,6]</sup> , 135.6 <sup>[3]</sup>
T <sub>dec.</sub> [°C]	1898 K (adiabatic dec. <i>T</i> , calcd., CHEETAH) <sup>[5]</sup>
ρ [g cm <sup>-3</sup> ]	0.933 (@ 298.15 K) <sup>[2,3,4]</sup>
Heat of formation	277.0 kJ/mol (Δ <sub>f</sub> H <sup>o</sup> ), 2,427 kJ/kg <sup>[3]</sup> , 586 cal/g <sup>[4]</sup> , 580 cal/g <sup>[3]</sup>
Heat of combustion	-28.77 kJ/g (exptl.) <sup>[5]</sup>

	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^{\circ} [\text{kJ kg}^{-1}]$	2,616		
$T_{\text{ex}} [\text{K}]$	2,054		
$p_{\text{CJ}} [\text{kbar}]$	75		
$\text{VoD} [\text{m s}^{-1}]$	5,778 (@ TMD)		
$V_0 [\text{L kg}^{-1}]$	910		

Koenen test	No change in steel sleeve for nozzle plate with 8 mm diameter hole, 60 mm height of DMAZ, after heating for 40 s, vapors vented from steel sleeve were ignited <sup>[5]</sup> , same results for nozzle plates containing holes of 5 mm, 3 mm or 2 mm diameter <sup>[5]</sup> , for nozzle plate containing hole with 1.5 mm diameter, after 46 s heating the DMAZ vapors were ignited to burn during 12 s, and steel sleeve exploded due to increase in internal pressure <sup>[5]</sup>																								
Initiation efficiency	Can be ignited using a conventional Shell 405 (iridium-based), catalyst bed preheated to ~ 150–200 °C <sup>[4]</sup> , shock wave from explosion of no. 8 detonator is not able to initiate DMAZ <sup>[5]</sup>																								
Card gap test	Negative (does not detonate) <sup>[4]</sup>																								
Flash point [°C]	29.4 <sup>[3,4]</sup>																								
Flammability	Lower flammability limit = 1.3 volume % in air <sup>[4]</sup> , UFL ≥ 22.4 vol. % in air <sup>[4]</sup>																								
Thermal stability	DMAZ concentration (wt.%) versus time (h) @ various $T$ (N <sub>2</sub> atmosphere, atmospheric pressure = 3 bar, moisture = 0.05 wt.%) <sup>[6]</sup> :																								
	<table border="1"> <thead> <tr> <th colspan="4"><math>T</math> (°C)</th> </tr> <tr> <th>60</th> <th>70</th> <th>80</th> <th>90</th> </tr> </thead> <tbody> <tr> <td>99.5%/300 h</td> <td>99%/300 h</td> <td>99%/200 h</td> <td>99%/100 h</td> </tr> <tr> <td>99.2/450</td> <td>96.5/500</td> <td>95.5/450</td> <td>96.5/200</td> </tr> <tr> <td>98.5/700</td> <td>96/550</td> <td>89/550</td> <td>94.5/275</td> </tr> <tr> <td>91.5/1050</td> <td>93.5/675</td> <td>82.5/625</td> <td></td> </tr> </tbody> </table> <p>Effect of N<sub>2</sub> pressure on DMAZ concentration (atmosphere = N<sub>2</sub>, moisture = 0.05 wt.%, <math>T</math> = 90 °C, <math>t</math> = 1,000 h, approx. values)<sup>[6]</sup>: 93.40 % @ 1.00 bar, 94.94 % @ 1.80 bar, 96.47 % @ 2.90 bar, 97.38 % @ 3.95 bar, 98.61 % @ 5.10 bar<sup>[6]</sup></p> <p>Est. shelf-life @ 25 °C = 67 m 780 h (7.73 years)<sup>[6]</sup></p>	$T$ (°C)				60	70	80	90	99.5%/300 h	99%/300 h	99%/200 h	99%/100 h	99.2/450	96.5/500	95.5/450	96.5/200	98.5/700	96/550	89/550	94.5/275	91.5/1050	93.5/675	82.5/625	
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91.5/1050	93.5/675	82.5/625																							
Vapor pressure [atm @ °C]	~0.8 bar @ 90 °C <sup>[6]</sup>																								

Viscosity [cP]	2 (@ 25 °C) <sup>[3,cited in 4]</sup> , 0.7034 (@ 25 °C) <sup>[4]</sup>																																			
Surface tension [dyne/cm]	25 (@ 25 °C) <sup>[4]</sup>																																			
Burn rate [mm/s]	Sensitivity to direct flame: ignited in all tests but no explosion <sup>[5]</sup>																																			
Solubility [g/mL]	Fully miscible with H <sub>2</sub> O but reacts to form nitric acid <sup>[4]</sup>																																			
Compatibility	Storing in glass vials for 20 days @ 60 °C: Monel, Inconel 600 and 300 series stainless steels showed some interaction with DMAZ but not severe dec. and PTFE showed good compatibility <sup>[4]</sup> , storing for 60 days @ 40 °C: 300 series stainless steels, titanium and aluminum showed slight interaction and PTFE showed good compatibility <sup>[4]</sup> , fully miscible with H <sub>2</sub> O but reacts to form nitric acid <sup>[4]</sup>																																			
$I_{sp}$ [s]	<p>Predicted performance using NTO as oxidizer: mixture ratio = 2.25, vacuum <math>I_{sp}</math> = 308.2 s, chamber <math>T</math> = 3528 K, chamber <math>H</math> = 144.9 cal/g, Mol. Wt. = 25.07, Ae/At = 9.795, C* = 1,700 m/s, Cf = 1.634<sup>[4]</sup></p> <p>Calcd. performance data @ engine operating pressure of 68 atm<sup>[3]</sup>:</p> <table border="1"> <thead> <tr> <th>Fuel/oxidizer</th> <th>Optimum O/F ratio</th> <th><math>d_{propellant}</math></th> <th>Optimum <math>I_{sp}</math> (s)</th> <th><math>D/I_{sp}</math> (s)</th> </tr> </thead> <tbody> <tr> <td>DMAZ/IRFNA</td> <td>2.5</td> <td>1.274</td> <td>272.7</td> <td>347.5</td> </tr> <tr> <td>DMAZ/HNO<sub>3</sub></td> <td>2.5</td> <td>1.278</td> <td>270.7</td> <td>346.4</td> </tr> <tr> <td>DMAZ/N<sub>2</sub>O<sub>4</sub></td> <td>2</td> <td>1.215</td> <td>283.1</td> <td>344</td> </tr> <tr> <td>DMAZ/MON-10</td> <td>2</td> <td>1.216</td> <td>283.3</td> <td>344.5</td> </tr> <tr> <td>DMAZ/H<sub>2</sub>O<sub>2</sub></td> <td>3.5</td> <td>1.283</td> <td>280.8</td> <td>360.2</td> </tr> <tr> <td>DMAZ/LOX</td> <td>1.5</td> <td>1.047</td> <td>305.8</td> <td>320.3</td> </tr> </tbody> </table>	Fuel/oxidizer	Optimum O/F ratio	$d_{propellant}$	Optimum $I_{sp}$ (s)	$D/I_{sp}$ (s)	DMAZ/IRFNA	2.5	1.274	272.7	347.5	DMAZ/HNO <sub>3</sub>	2.5	1.278	270.7	346.4	DMAZ/N <sub>2</sub> O <sub>4</sub>	2	1.215	283.1	344	DMAZ/MON-10	2	1.216	283.3	344.5	DMAZ/H <sub>2</sub> O <sub>2</sub>	3.5	1.283	280.8	360.2	DMAZ/LOX	1.5	1.047	305.8	320.3
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$D/I_{sp}$	13.77 lbf*s/in <sup>3[3]</sup>																																			
Heat of dec. [kJ/g]	-22.75 <sup>[3]</sup> , -3.896 (max. heat of dec., calcd. CHEETAH) <sup>[5]</sup> , -22.75 (heat of dec., calcd. CHEETAH) <sup>[5]</sup>																																			

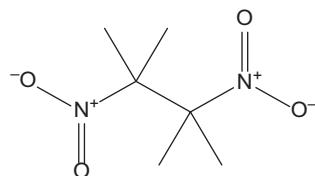
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## 2,3-Dimethyl-2,3-dinitrobutane

Name [German, acronym]: 2,3-Dimethyl-2,3-dinitrobutane [DMDNB, DMNB]

Main (potential) use: Taggant, detection agent for explosives<sup>[4]</sup>, one of four possible detection taggants that must be added to explosives according to the Int. Civil Aviation Organization<sup>[5]</sup>

Structural formula:



	<b>DMDNB</b>															
Formula	C <sub>6</sub> H <sub>12</sub> N <sub>2</sub> O <sub>4</sub>															
Molecular mass [g mol <sup>-1</sup> ]	176.1720															
Appearance at RT																
IS [J]	40 (<100 µm)															
FS [N]	360 (<100 µm)															
ESD [J]	1.5 (<100 µm)															
N [%]	15.90															
Ω(CO <sub>2</sub> ) [%]	-127.15															
T <sub>phase transition</sub> [°C]	<p>322 K (onset, rotational transition, <i>gauche</i> → <i>trans</i>, reversible, DTA)<sup>[4]</sup>, 388 K (onset, crystalline transformation from triclinic to body-centered cubic, reversible, DTA)<sup>[4]</sup></p> <p>Onset <i>T</i>, DSC, values independent of heating rates between 1 and 10 K/min, both reversible transitions<sup>[4]</sup>:</p> <table border="1"> <thead> <tr> <th>Transition</th><th><i>T</i> (K)</th><th>Δ<i>H</i> (kJ/mol)</th><th>Δ<i>S</i> (JK<sup>-1</sup> mol<sup>-1</sup>)</th><th>Hysteresis width (K)</th></tr> </thead> <tbody> <tr> <td>I→II (<i>gauche</i> → <i>trans</i>)</td><td>321 ± 2</td><td>1.0 ± 0.2</td><td>3.5 ± 0.7</td><td>13 ± 2</td></tr> <tr> <td>II→III (triclinic → bcc)</td><td>388 ± 2</td><td>18.1 ± 1.5</td><td>46.4 ± 3.9</td><td>17 ± 4</td></tr> </tbody> </table>	Transition	<i>T</i> (K)	Δ <i>H</i> (kJ/mol)	Δ <i>S</i> (JK <sup>-1</sup> mol <sup>-1</sup> )	Hysteresis width (K)	I→II ( <i>gauche</i> → <i>trans</i> )	321 ± 2	1.0 ± 0.2	3.5 ± 0.7	13 ± 2	II→III (triclinic → bcc)	388 ± 2	18.1 ± 1.5	46.4 ± 3.9	17 ± 4
Transition	<i>T</i> (K)	Δ <i>H</i> (kJ/mol)	Δ <i>S</i> (JK <sup>-1</sup> mol <sup>-1</sup> )	Hysteresis width (K)												
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	DSC results, T onset sealed glass capillaries <sup>[4]</sup> :		
	Heating rate (K/min)	T (K)	$\Delta H$ (kJ/mol)
	2.02	387	19.2
	4.04	388	15.9
	6.07	388	19.4
	8.09	388	17.5
	10.13	388	18.7
	Average		18.1 ± 1.5
$T_{m.p.}$ [°C]	200 (sealed glass ampule), 475 (DSC @ 8 K/min) <sup>[4]</sup> , 480 ± 5 K <sup>[4]</sup>		
	DSC results <sup>[4]</sup> :		
	Heating rate (K/min)	Fusion T (K)	$\Delta H$ (kJ/mol)
	2.02	476	3.4
	4.04	480	5.8
	6.07	483	6.7
	8.09	484	6.5
	10.13	486	7.4
$T_{dec}$ [°C]	227 (sealed glass ampule) (DSC @ 5 °C/min),		
	DSC results <sup>[4]</sup> :		
	Heating rate (K/min)	Dec. (exotherm) T (K)	$\Delta H$ (kJ/mol)
	2.02	513	577
	4.04	520	482
	6.07	526	591
	8.09	529	523
	10.13	532	539
	Average		542 ± 44
$\rho$ [g cm <sup>-3</sup> ]	1.430 (@ 95 K), 1.388 (@ 298 K)		
Heat of formation	-311 ± 1 kJ/mol ( $\Delta_f H^\circ$ , (s)) <sup>[1]</sup> , -311.0 kJ/mol (enthalpy of form., exptl.) <sup>[6]</sup> , -333.3 kJ/mol (enthalpy of form., calcd., emp.) <sup>[6]</sup> , -326 kJ/mol (enthalpy of form., calcd., S-D method) <sup>[6]</sup>		
Heat of combustion	-3,765 ± 1 kJ/mol ( $\Delta_c H^\circ$ , solid) <sup>[1]</sup> , -3,855 ± 6.7 kJ/mol ( $\Delta_c H^\circ$ , solid) <sup>[1]</sup>		
	Calcd. (EXPLO5 6.03)		Exptl.
$-\Delta_{ex} U^\circ$ [kJ kg <sup>-1</sup> ]	3,116		

$T_{\text{ex}}$ [K]	2,063	
$p_{\text{C}_1}$ [kbar]	132	
VoD [ $\text{m s}^{-1}$ ]	6,398 (@ TMD)	
$V_0$ [ $\text{L kg}^{-1}$ ]	820	

Solubility [g/mL]	Soluble in $\text{CCl}_4^{[4]}$ , soluble in mesitylene <sup>[4]</sup>																						
Enthalpy of sublimation [kJ/mol]	$94 \pm 1^{[4]}$																						
Enthalpy of fusion [kJ/mol]	$20 \pm 6^{[4]}$ , $\Delta_{\text{fus}}H(298 \text{ K}) = 14.9 \pm 3.4$ (calcd. from $\Delta H$ of (s) and (l)) <sup>[4]</sup> DSC results <sup>[4]</sup> : <table border="1"> <thead> <tr> <th>Heating rate (K/min)</th> <th>Fusion <math>T</math> (K)</th> <th><math>\Delta H</math> (kJ/mol)</th> </tr> </thead> <tbody> <tr> <td>2.02</td> <td>476</td> <td>3.4</td> </tr> <tr> <td>4.04</td> <td>480</td> <td>5.8</td> </tr> <tr> <td>6.07</td> <td>483</td> <td>6.7</td> </tr> <tr> <td>8.09</td> <td>484</td> <td>6.5</td> </tr> <tr> <td>10.13</td> <td>486</td> <td>7.4</td> </tr> </tbody> </table>		Heating rate (K/min)	Fusion $T$ (K)	$\Delta H$ (kJ/mol)	2.02	476	3.4	4.04	480	5.8	6.07	483	6.7	8.09	484	6.5	10.13	486	7.4			
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Average		542 $\pm$ 44																					

	DMDNB <sup>[2]</sup>	DMDNB <sup>[2]</sup>	DMDNB <sup>[3]</sup>	DMDNB <sup>[3]</sup>
Chemical formula	$\text{C}_6\text{H}_{12}\text{N}_2\text{O}_4$	$\text{C}_6\text{H}_{12}\text{N}_2\text{O}_4$	$\text{C}_6\text{H}_{12}\text{N}_2\text{O}_4$	$\text{C}_6\text{H}_{12}\text{N}_2\text{O}_4$
Molecular weight [g mol <sup>-1</sup> ]	176.17	176.17	176.17	176.17
Crystal system	Triclinic	Triclinic		
Space group	<i>P</i> -1 (no. 2)	<i>P</i> -1 (no. 2)		
<i>a</i> [\AA]	6.300(5)	6.371(2)	6.84	7.89
<i>b</i> [\AA]	6.380(3)	6.535(2)	6.63	7.89
<i>c</i> [\AA]	11.851(9)	12.353(4)	12.62	7.89

$\alpha$ [°]	100.73(6)	103.31(4)	107.0	90
$\beta$ [°]	81.00(6)	79.31(4)	94.8	90
$\gamma$ [°]	118.72(5)	119.84(3)	59.0	90
$V$ [Å <sup>3</sup> ]	409.194	432.603	467.562	491.169
$Z$	2	2	2	2
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.43	1.351	1.251	1.191
$T$ [K]	95	295	295	295

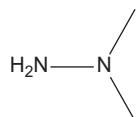
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**(Unsymmetrical) dimethylhydrazine**

Name [German, acronym]: 1,1-Dimethylhydrazine, *unsym*-dimethylhydrazine, *asym*-dimethylhydrazine, *N,N*-dimethylhydrazine, dimazine [dimethylhydrazin, UDMH]

Main (potential) use: In hypergolic liquid-fuel rockets<sup>[1]</sup>

Structural formula:



	<b>UDMH</b>
Formula	C <sub>2</sub> H <sub>8</sub> N <sub>2</sub>
Molecular mass [g mol <sup>-1</sup> ]	60.10
Appearance at RT	Colorless liquid <sup>[6,9]</sup> , flammable, colorless, mobile liquid <sup>[11]</sup>
N [%]	46.61
Ω(CO <sub>2</sub> ) [%]	-213.0
T <sub>m.p.</sub> [°C]	-57.2 <sup>[1,2]</sup> , -57 <sup>[8]</sup> , -57.7 (freezing point) <sup>[9]</sup> , -57.21 (freezing point) <sup>[10]</sup> , -58 <sup>[11]</sup> , -57 (freezing point) <sup>[12]</sup>
T <sub>b.p.</sub> [°C]	64 <sup>[8]</sup> , 63.3 <sup>[9]</sup> , 63 <sup>[10]</sup> , bp <sub>760</sub> = 63.9 <sup>[11]</sup>
ρ [g cm <sup>-3</sup> ]	0.786 <sup>[1,10]</sup> , 0.786 (@ 298.15 K) <sup>[3]</sup> , 0.7861 (@ 25 °C) <sup>[8]</sup> , 0.790 (@ 15.6 °C) <sup>[5]</sup> , 0.784 (@ 25 °C) <sup>[6]</sup> , d <sup>22</sup> <sub>4</sub> = 0.791 <sup>[11]</sup> , d <sup>25</sup> <sub>25</sub> = 0.782 <sup>[11]</sup> , n <sup>22.3</sup> <sub>D</sub> = 1.40753 <sup>[11]</sup> , 0.78 <sup>[12]</sup>
Heat of formation	85.3 kJ/mol (Δ <sub>f</sub> H <sup>o</sup> ) <sup>[4]</sup> , 1419.3 kJ kg <sup>-1</sup> (Δ <sub>f</sub> H <sup>o</sup> ) <sup>[4]</sup> , +828 kJ/kg (enthalpy of form.) <sup>[1]</sup> , 12.74 kcal/mol (@ 25 °C) <sup>[6]</sup> , 19.92 kcal/mol (Δ <sub>f</sub> H (g), exptl.) <sup>[7]</sup> , +11.9 kcal/mol (heat of form. @ 298.15 K) <sup>[10]</sup> , +48.83 kJ/mol (enthalpy of form.) <sup>[8]</sup> , 48.9 ± 3.2 kJ/mol (liq., Δ <sub>f</sub> H <sup>o</sup> ) <sup>[13]</sup> , 83.9 ± 3.2 kJ/mol (gaseous, Δ <sub>f</sub> H <sup>o</sup> ) <sup>[13]</sup>
Heat of combustion	474.11 kcal/mol <sup>[6]</sup>
	Calcd. (EXPLO5 6.04)
	Exptl.
-Δ <sub>ex</sub> U <sup>o</sup> [kJ kg <sup>-1</sup> ]	3,183
T <sub>ex</sub> [K]	1,713
p <sub>C-J</sub> [GPa]	7.5

VoD [m s <sup>-1</sup> ]	6,076 (@ 0.827 g cm <sup>-3</sup> , Δ <sub>f</sub> H = 53 kJ mol <sup>-1</sup> )	
V <sub>0</sub> [L kg <sup>-1</sup> ]	1,123	
I <sub>s</sub> [s]	280.0 <sup>[12]</sup> , I <sub>d</sub> = 388.0 <sup>[12]</sup>	

Critical temperature [°C]	249 <sup>[10]</sup>
Critical pressure [atm]	60 <sup>[10]</sup>
5 s explosion T [°C] Ignition T [°C]	250 (spontaneous ignition T) <sup>[9]</sup>
Flash point [°C]	1.1 <sup>[9]</sup>
Vapor pressure [atm @ °C]	157 mm (@ 25 °C) <sup>[6]</sup> , 160 mm Hg (@ 26.7 °C) <sup>[5]</sup> , 20.9 kPa @ 25 °C <sup>[8]</sup> , 2.3668 (units not specified) @ 25 °C <sup>[10]</sup>
Solubility [g/mL]	Very soluble in water, EtOH and most petroleum fuels <sup>[9]</sup> , miscible with water with evolution of heat <sup>[11]</sup> , miscible with EtOH, Et <sub>2</sub> O, DMF, hydrocarbons <sup>[11]</sup>
Viscosity (cP)	0.51 (@ 25 °C) <sup>[6]</sup> , 0.509 (@ 25 °C) <sup>[10]</sup>
Hygroscopicity	Hygroscopic – fumes in air and gradually turns yellow <sup>[11]</sup>
Compatibility	Hypergolic with some oxidants, for example, fuming nitric acid <sup>[9]</sup> , storage and shipment equipment is made of mild steel <sup>[9]</sup> , compatible with most common metals and can be handled in containers of those metals under a variety of conditions <sup>[10]</sup> , no known limitation on use of Ni, Monel, stainless steel (types 303, 304, 316, 321 and 347) <sup>[10]</sup> , Al is attacked to some extent by dilute aqueous UDMH solns. <sup>[10]</sup> , incompatible with Cu or Cu alloys <sup>[10]</sup> , fumes in air and gradually turns yellow <sup>[11]</sup>
Heat of vaporization [kcal/mol]	8.366 @ 25 °C <sup>[10]</sup>
Specific heat [cal/g°C]	0.6526 @ 25 °C <sup>[10]</sup>

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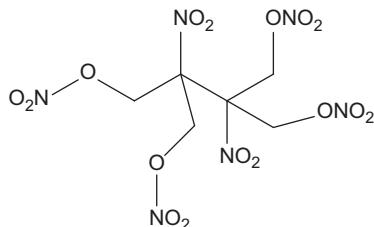
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## 1,4-Dinitrato-2,3-dinitro-2,3-bis(nitratomethylene)butane

Name [German, acronym]: 3,4-Dideoxy-3,4-dinitro-1,2,5,6-tetra-o-nitrohexitol, 1,4-dinitrato-2,3-dinitro-2,3-bis(nitratomethylene) butane, 2,3-dinitro-2,3-bis((nitrooxy)methyl)-butane-1,4-diyl dinitrate, nitrate ester-1, 2,3-Bis(hydroxymethyl)-2,3-dinitro-1,4-butanediol tetranitrate, 2,2-bis(nitroxymethyl)-2,3-dinitrobutane-1,4-diol dinitrate [3,4-dideoxy-3,4-dinitro-1,2,5,6-tetra-o-nitrohexitol, 1,4-dinitrato-2,3-dinitro-2,3-bis(nitratromethylene) butan, SMX, DNTN, BHDBT, NEST-1]

Main (potential) use: Potential component for propellants<sup>[2]</sup>, (highest density of all known nitrate esters up to the year 2018)<sup>[2]</sup>, high-energy-density melttable explosive<sup>[4]</sup>, possible new melt-castable secondary explosive<sup>[1,6]</sup>, potential as solid propellant ingredient<sup>[8]</sup>

Structural formula:



	DNTN
Formula	C <sub>6</sub> H <sub>8</sub> N <sub>6</sub> O <sub>16</sub>
Molecular mass [g mol <sup>-1</sup> ]	420.18
Appearance at RT	Colorless fine crystalline powder <sup>[2]</sup> , white crystalline substance <sup>[4]</sup> , white solid <sup>[5]</sup> , colorless crystals, white solid <sup>[1]</sup>
IS [J]	$H_{50} = 10.0 \text{ cm}$ (5 kg mass) <sup>[3]</sup> , similar to that of PETN <sup>[4]</sup> , $DH_{50} = 27.7 \text{ cm}$ (4 kg mass, Bruceton method, 35 mg sample, 120 grit sandpaper, LLNL small-scale apparatus) <sup>[5]</sup> , 2.7 <sup>[6]</sup> , comparable to PETN <sup>[6,8]</sup> , $H_{50\%} = 11 \text{ cm}$ (2.5 kg mass, LANL type 12) <sup>[7]</sup> , 2.7 (2.5 kg mass, 50% initiation level, LANL type 12) <sup>[1]</sup> , 4.9 (ERL method 1012) <sup>[8]</sup>

FS [N]	$p_0 = 240$ MPa (pendulum, drop hammer K-44-II, lower limit, $p_0$ = no explosions in 20 parallel experiments) <sup>[2]</sup> , $p_{50} = 260$ MPa (pendulum, drop hammer K-44-II, lower limit, $p_{50}$ = 50% explosions in 20 parallel experiments) (cf. $p_0 = 170$ MPa, $p_{50} = 300$ MPa for PETN) <sup>[2]</sup> , 100% (3.92 MPa, 90 °) <sup>[3]</sup> , comparable to that of octogen <sup>[4]</sup> , 74.5 <sup>[6]</sup> , comparable to PETN <sup>[6,8]</sup> , 7.6 kg (50% load, Bruceton method) <sup>[7]</sup> , 74.5 (50% load, Bruceton method) <sup>[1]</sup> , 75 (BAM method 1024) <sup>[8]</sup>																																																												
ESD [J]	0.625 <sup>[6]</sup> , comparable to PETN <sup>[6,8]</sup> , 0.0625 (ABL spark threshold initiation level) <sup>[7]</sup> , 0.625 (ABL spark threshold initiation level) <sup>[1]</sup> , 172 mJ (ARDEC method 1032) <sup>[8]</sup>																																																												
N [%]	20.0																																																												
$\Omega(\text{CO}_2)$ [%]	0																																																												
$T_{\text{m.p.}}$ [°C]	85–86 <sup>[1,4,5,6,7]</sup> , 81 (SDTA @ 10 °C/min) <sup>[2]</sup> , 86.38 (DSC/TG) <sup>[3]</sup> , 84.4–86.3 (DTA @ 5 °C/min) <sup>[4]</sup> , 82 (crude product) <sup>[4]</sup> , 84–86 (recryst. from isopropyl alcohol) <sup>[4]</sup> , 81–84 (crude product) <sup>[5]</sup> , 84–85 (recryst. from EtOH) <sup>[5]</sup> , 85 (onset, DSC @ 10 °C/min) <sup>[8]</sup>  DSC, flame sealed in glass microampules, N <sub>2</sub> @ 50 mL/min <sup>[5]</sup> :																																																												
	<table border="1"> <thead> <tr> <th>Heating rate (K/min)</th> <th><i>n</i></th> <th>Mass (mg)</th> <th>Endotherm, <math>T_{\text{min}}</math> (°C)</th> <th><math>\Delta H_{\text{fus}}</math> (J/g)</th> </tr> </thead> <tbody> <tr><td>20</td><td>4</td><td>0.311</td><td>88</td><td>135</td></tr> <tr><td>10</td><td>3</td><td>0.279</td><td>87</td><td>71</td></tr> <tr><td>9</td><td>2</td><td>0.381</td><td>87</td><td>99</td></tr> <tr><td>8</td><td>3</td><td>0.338</td><td>86</td><td>70</td></tr> <tr><td>7</td><td>2</td><td>0.354</td><td>85</td><td>50</td></tr> <tr><td>6</td><td>1</td><td>0.313</td><td>85</td><td>80</td></tr> <tr><td>5</td><td>3</td><td>0.223</td><td>84</td><td>70</td></tr> <tr><td>4</td><td>3</td><td>0.433</td><td>85</td><td>80</td></tr> <tr><td>3</td><td>2</td><td>0.400</td><td>86</td><td>89</td></tr> <tr><td>2</td><td>3</td><td>0.311</td><td>86</td><td>87</td></tr> <tr><td>1</td><td>3</td><td>0.250</td><td>84</td><td>81</td></tr> </tbody> </table>	Heating rate (K/min)	<i>n</i>	Mass (mg)	Endotherm, $T_{\text{min}}$ (°C)	$\Delta H_{\text{fus}}$ (J/g)	20	4	0.311	88	135	10	3	0.279	87	71	9	2	0.381	87	99	8	3	0.338	86	70	7	2	0.354	85	50	6	1	0.313	85	80	5	3	0.223	84	70	4	3	0.433	85	80	3	2	0.400	86	89	2	3	0.311	86	87	1	3	0.250	84	81
Heating rate (K/min)	<i>n</i>	Mass (mg)	Endotherm, $T_{\text{min}}$ (°C)	$\Delta H_{\text{fus}}$ (J/g)																																																									
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$T_{\text{evaporation}}$ [°C]	85–145 (SDTA @ 10 °C/min) <sup>[2]</sup>																																																												
$T_{\text{dec.}}$ [°C]	Exothermic peak $T_{\text{dec.}}$ versus heating rate, closed cell, <1 mm hole diameter <sup>[2]</sup> :  <table border="1"> <thead> <tr> <th>Heating rate (°C/min)</th> <th><math>T_{\text{dec. peak}}</math> T (°C)</th> </tr> </thead> <tbody> <tr><td>5</td><td>178</td></tr> <tr><td>10</td><td>187</td></tr> <tr><td>15</td><td>192</td></tr> <tr><td>20</td><td>197</td></tr> </tbody> </table>	Heating rate (°C/min)	$T_{\text{dec. peak}}$ T (°C)	5	178	10	187	15	192	20	197																																																		
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	154 (onset) <sup>[2]</sup> , 145–210 (TGA/SDTA @ 10 °C/min) <sup>[2]</sup> , 185.79 (DSC/TG) <sup>[3]</sup> , 143 (initial dec. $T$ , DTA @ 5 °C/min) <sup>[4]</sup> , 160 (onset of extensive thermal degradation, DTA @ 5 °C/min), 174.0 (exo peak max, DTA 5 °C/min) <sup>[4]</sup> , 141 <sup>[6]</sup> , 183 (DSC @ 10 °C/min) <sup>[7]</sup> , 141 (onset) (DSC @ 10 °C/min) <sup>[1]</sup> , 140 (exo, onset, DSC @ 10 °C/min) <sup>[8]</sup>					
	DSC, flame sealed in glass microampules, N <sub>2</sub> @ 50 mL/min <sup>[5]</sup> :					
Heating rate (K/min)	<i>n</i>	Mass (mg)	Exotherm, <i>T</i> <sub>min</sub> (°C)	Exotherm, <i>T</i> <sub>max</sub> (°C)	Δ <i>H</i> (J/g)	
20	4	0.311	179	185	3,185	
10	3	0.279	170	175	3,121	
9	2	0.381	167	171	3,756	
8	3	0.338	165	169	3,116	
7	2	0.354	166	169	2,730	
6	1	0.313	163	167	3,855	
5	3	0.223	159	163	2,809	
4	3	0.433	155	158	3,934	
3	2	0.400	150	154	3,342	
2	3	0.311	151	149	3,257	
1	3	0.250	154	142	3,342	
	180 (max. mass loss, @ 10 K/min, DTA) <sup>[5]</sup>					
ρ [g cm <sup>-3</sup> ]	1.917 <sup>[1,6]</sup> , 1.917 (@ 103 K, X-ray) <sup>[1,cited in 4,5]</sup> , 1.856 (flotation method, @ 20 °C, crystals from obtained from CH <sub>2</sub> Cl <sub>2</sub> /hexane) <sup>[4]</sup> , 1.823 (flotation method, @ 20 °C, crystals from isopropyl alcohol) <sup>[4]</sup> , 1.8238 <sup>[4]</sup> , 1.8238 ± 0.0016 (pycnometer) <sup>[5]</sup> ,					
Heat of formation	−497.8 kJ/mol (calcd.,) <sup>[2]</sup> , −371 (Δ <i>H</i> <sup>0</sup> <sub>f</sub> ) <sup>[4,6]</sup> , −371.00 kJ/mol <sup>[5]</sup> , −371 kJ/mol (combustion calorimetry) <sup>[1]</sup>					
	Calcd. (EXPLO5 6.04)	Lit. values			Exptl.	
−Δ <sub>ex</sub> <i>U</i> <sup>0</sup> [kJ kg <sup>-1</sup> ]						
<i>T</i> <sub>ex</sub> [K]						
<i>p</i> <sub>C-J</sub> [kbar]		34.97 GPa (@ 1.8238 g cm <sup>-3</sup> (pycnometry density), heat of formation = −371.0 kJ/mol, CHEETAH 6.0) <sup>[5]</sup>				

		3.597 GPa (@ 0.69 g cm <sup>-3</sup> (SSED density), heat of formation = -371.0 kJ/mol, CHEETAH 6.0) <sup>[5]</sup>  400 (calcd.) <sup>[6]</sup>  40 GPa (@ 1.917 g cm <sup>-3</sup> , ΔH <sub>f</sub> = -371 kJ/mol, calcd., CHEETAH 5.0) <sup>[1,7]</sup>															
VoD [m s <sup>-1</sup> ]		8,895 (@ 1.8238 g cm <sup>-3</sup> (pycometry density), heat of formation = -371.0 kJ/mol, CHEETAH 6.0) <sup>[5]</sup>  4,187 (@ 0.69 g cm <sup>-3</sup> (SSED density), heat of formation = -371.0 kJ/mol, CHEETAH 6.0) <sup>[5]</sup>  9,100 (calcd.) <sup>[6]</sup>  9,100 (@ 1.917 g cm <sup>-3</sup> , ΔH <sub>f</sub> = -371 kJ/mol; calcd., CHEETAH 5.0) <sup>[1,7]</sup>															
V <sub>0</sub> [L kg <sup>-1</sup> ]																	
Thermal stability	$\tau_{0.02\%}$ = 18 days required (@ 20 °C, calcd., cf. hundreds of years for HMX and RDX) <sup>[2]</sup> Amount of dec. as a function of time in closed cell, 1 mm hole @ 90 °C <sup>[2]</sup> : <table border="1"> <thead> <tr> <th>Heating time (min)</th> <th>Decomposed SMX (%)</th> </tr> </thead> <tbody> <tr> <td>1</td> <td>0.013</td> </tr> <tr> <td>5</td> <td>0.065</td> </tr> <tr> <td>10</td> <td>0.13</td> </tr> <tr> <td>15</td> <td>0.2</td> </tr> <tr> <td>30</td> <td>0.4</td> </tr> <tr> <td>60</td> <td>0.8</td> </tr> </tbody> </table> ~ 4 wt.% mass loss in open cell @ 90 °C in 60 min <sup>[2]</sup> , evaporation and decomposition occur on heating SMX, SMX evaporates faster than it decomposes <sup>[2]</sup>			Heating time (min)	Decomposed SMX (%)	1	0.013	5	0.065	10	0.13	15	0.2	30	0.4	60	0.8
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Vapor pressure [atm @ °C]	4.10 × 10 <sup>-3</sup> Pa @ 25 °C <sup>[5]</sup>																

Burn rate [mm/s]	Data from ref. <sup>[2]</sup>
	<p>Fig. 7: The influence of catalyst on the burning rate of SMX: 1 – SMX, 2 – SMX + 3% CLP + 1.5% C.</p>
Solubility [g/mL]	Easily soluble in organochlorine solvents (e.g., CH <sub>2</sub> Cl <sub>2</sub> , dichloroethane), acetone and EtOH <sup>[4]</sup> , insoluble in hydrocarbons (e.g., hexane) <sup>[4]</sup> , soluble in EtOH, MeOH, 2-propanol, acetone and acetonitrile <sup>[5]</sup> , can be recryst. from a wide range of common organic solvents <sup>[1]</sup> , large hexagonal crystals from EtOH, isopropanol <sup>[1]</sup>
Explosive energy [kJ/ cm <sup>3</sup> ]	4.747 <sup>[2]</sup>
Shock velocity [km/s]	9.287 <sup>[2]</sup>
Activation energy to thermal decomposition [kJ/mol]	133.2 <sup>[2]</sup>
ΔH <sub>melt</sub> [J/g]	183.27 (DTA @ 5 °C/min) <sup>[4]</sup>
ΔH <sub>dec</sub> [J/g]	2,931.8 (DTA @ 5 °C/min) <sup>[4]</sup> , 2,237 <sup>[7]</sup> , 1,818 (heat of dec.) <sup>[1]</sup>
ΔH <sub>sub</sub> [kJ/mol]	105.3 <sup>[5]</sup>

Small-scale explosivity device (SSED)	British.303 cartridge, 2 g explosive, RP-3 EBW <sup>[5]</sup> :				
	Charge depth (mm)	Tap density (g mL <sup>-1</sup> )	Mass cartridge (g)	Mass remaining (g)	Fraction remaining (%)
	21	0.77	11.1826	2.7519	24.6
	17	0.69	11.1314	2.9157	26.2
	20	0.77	11.4555	2.9974	26.2
	26	0.91	11.3384	2.7119	23.9
<i>t</i> <sub>sp</sub> [s]	254.96 (calcd., CHEETAH) <sup>[7]</sup>				
Thermal properties	(thermal conductivity) $k = 0.266 \pm 0.005 \text{ W}(\text{m} - \text{K})^{-1}$ <sup>[8]</sup> , (thermal diffusivity) $\alpha = 0.118 \pm 0.006 \text{ mm}^2 \text{ s}^{-1}$ <sup>[8]</sup>				

	3,4-Dideoxy-3,4-dinitro-1,2,5,6-tetra- <i>o</i> -nitrohexitol <sup>[1]</sup>	BHDBT <sup>[3]</sup>	2,3-Bis(nitroxymethyl)-2,3-dinitrobutane-1,4-diol dinitrate <sup>[4]</sup>
Chemical formula	C <sub>6</sub> H <sub>8</sub> N <sub>6</sub> O <sub>16</sub>	C <sub>6</sub> H <sub>8</sub> N <sub>6</sub> O <sub>16</sub>	C <sub>6</sub> H <sub>8</sub> N <sub>6</sub> O <sub>16</sub>
Molecular weight [g mol <sup>-1</sup> ]	420.18	420.18	420.18
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	<i>P</i> 2 <sub>1</sub> / <i>n</i>	<i>P</i> 2 <sub>1</sub> / <i>n</i>	<i>P</i> 2 <sub>1</sub> / <i>n</i>
<i>a</i> [\AA]	8.1228(6)	8.1944(11)	8.1377(8)
<i>b</i> [\AA]	23.0560(16)	23.365(3)	23.113(2)
<i>c</i> [\AA]	8.5072(6)	8.5838(11)	8.5220(9)
$\alpha$ [°]	90	90	90
$\beta$ [°]	113.9530(10)	113.501(2)	113.872(10)
$\gamma$ [°]	90	90	90
<i>V</i> [\AA <sup>3</sup> ]	1,456.01(18)	1,507.2(3)	465.7(3)
<i>Z</i>	4	4	4
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.917	1.852	1.904
<i>T</i> [K]	103	296	150

SMX powder from manufacturer has mean particle size of approx. 90 µm (optical microscopy)<sup>[8]</sup>, particles range from needle-like to jagged morphology typical for crystals obtained from 2-propanol solution<sup>[8]</sup>.

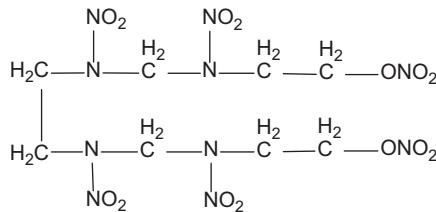
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- [7] M. C. Schulze, D. E. Chavez, *J. Energet. Mater.*, **2016**, *34*, 129–137.
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## 1,12-Dinitrato-3,5,8,10-tetranitrazadodecane

Name [German, acronym]: 1,12-Dinitrato-3,5,8,10-tetranitrazadodecane [TENA-2]

Main (potential) use: An example of a NENA compound which is a possible energetic plasticizer and component of explosives and propellant charge

Structural formula:



	TENA-2		
Formula	$\text{C}_8\text{H}_{16}\text{N}_{10}\text{O}_{14}$		
Molecular mass [g mol <sup>-1</sup> ]	476.27		
Appearance at RT			
IS [J]	10 Nm (5 kg mass, BAM) <sup>[1]</sup> , 10 Nm (1 kg mass, BAM) <sup>[2]</sup>		
FS [N]	32 kp (Julius-Peters) <sup>[1]</sup> , 32 kp (BAM) <sup>[2]</sup>		
N [%]	29.41		
$\Omega(\text{CO}_2)$ [%]	-33.6		
$T_{\text{m.p.}}$ [°C]	147 (endo peak, DTA/TG @ 6 K/min) <sup>[1,2]</sup>		
$T_{\text{dec.}}$ [°C]	~210 (exo peak, DTA/TG @ 6 K/min) <sup>[1,2]</sup>		
$\rho$ [g cm <sup>-3</sup> ]	1.73 (gas pycnometry) <sup>[1]</sup>		
Heat of formation	-101 kJ/mol ( $\Delta_f H^\circ$ , measured) <sup>[1]</sup>		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{\text{ex}} U^\circ$ [kJ kg <sup>-1</sup> ]			
$T_{\text{ex}}$ [K]			
$p_{\text{CJ}}$ [kbar]			

VoD [ $\text{m s}^{-1}$ ]		8,324 (@ 1.78 g $\text{cm}^{-3}$ , calcd., Rothstein) <sup>[1]</sup>  8,473 (@ 1.78 g $\text{cm}^{-3}$ , calcd., Kamlet) <sup>[1]</sup>	
$V_0$ [ $\text{L kg}^{-1}$ ]			

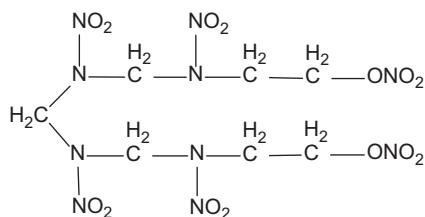
- [1] H. Ritter, M. R. Schäfer, B. Wanders, H. H. Licht, *Synthesis and Explosive Properties of Insensitive Energetic NENA Explosives*, ICT 2000, Karlsruhe, Germany, pp. 14-1–14-12.
- [2] H. Ritter, S. Braun, B. Wanders, *Synthesis and Sensitivity of Polynitramines*, ICT 2005, Karlsruhe, Germany, pp. 60-1–60-10.

## 1,11-Dinitrato-3,5,7,9-tetranitrazaundecane

Name [German, acronym]: 1,11-Dinitrato-3,5,7,9-tetranitrazaundecane [TENA-1]

Main (potential) use: An example of a NENA compound which is a possible energetic plasticizer and component of explosives and propellant charge

Structural formula:



	TENA-1		
Formula	$C_7H_{14}N_{10}O_{14}$		
Molecular mass [g mol <sup>-1</sup> ]	462.25		
Appearance at RT			
IS [J]	>25 Nm (5 kg mass, BAM) <sup>[1]</sup> , >25 (1 kg mass, BAM) <sup>[2]</sup>		
FS [N]	>36 kp (Julius-Peters) <sup>[1]</sup> , >36 kp (BAM) <sup>[2]</sup>		
N [%]	30.30		
$\Omega(CO_2)$ [%]	-24.2		
$T_{m.p.}$ [°C]	165 (endo, DTA/TG @ 6 K/min) <sup>[1]</sup> , 163 (DSC @ 5 K/min) <sup>[2]</sup>		
$T_{\text{phase transition}}$ [°C]	130 (small endo, crystal change, DTA/TG @ 6 K/min) <sup>[1]</sup>		
$T_{\text{dec.}}$ [°C]	~205 (exo peak max, DTA/TG @ 6 K/min) <sup>[1]</sup> , 200 (DSC @ 5 K/min) <sup>[2]</sup>		
$\rho$ [g cm <sup>-3</sup> ]	1.60 (gas pycnometry) <sup>[1]</sup>		
Heat of formation	-100 kJ/mol ( $\Delta_f H^\circ$ , est. based on known value of TENA-2) <sup>[1]</sup>		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^\circ$ [kJ kg <sup>-1</sup> ]			
$T_{\text{ex}}$ [K]			
$p_{\text{C-J}}$ [kbar]			

VoD [ $\text{m s}^{-1}$ ]		8,613 (@ 1.69 $\text{g cm}^{-3}$ , calcd., <i>Rothstein</i> ) <sup>[1]</sup>  8,212 (@ 1.69 $\text{g cm}^{-3}$ , calcd., <i>Kamlet</i> ) <sup>[1]</sup>	
$V_0$ [ $\text{L kg}^{-1}$ ]			

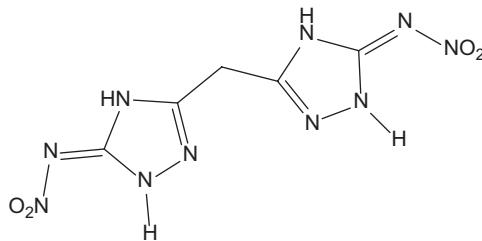
- [1] H. Ritter, M. R. Schäfer, B. Wanders, H. H. Licht, *Synthesis and Explosive Properties of Insensitive Energetic NENA Explosives*, ICT 2000, Karlsruhe, Germany, pp. 14-1 – 14-12.
- [2] H. Ritter, S. Braun, B. Wanders, *Synthesis and Sensitivity of Polynitramines*, ICT 2005, Karlsruhe, Germany, pp. 60-1 – 60-10.

## 5,5'-Dinitrimino-3,3'-methylene-1*H*-1,2,4-triazole

Name [German, acronym]: 5,5'-Dinitrimino-3,3'-methylene-1*H*-1,2,4-triazole  
 [5,5'-dinitrimino-3,3'-methylene-1*H*-1,2,4-triazol,  
 DNBTM]

Main (potential) use: Can act as sensitizer in LA systems<sup>[1]</sup>, too sensitive for use without some type of phlegmatizer<sup>[1]</sup>, potential new metal-free primary explosive with high thermal stability<sup>[2]</sup>

Structural formula:



	<b>DNBTM</b>		
Formula	C <sub>5</sub> H <sub>6</sub> N <sub>10</sub> O <sub>4</sub>		
Molecular mass [g mol <sup>-1</sup> ]	270.17		
Appearance at RT	Colorless solid <sup>[2]</sup>		
IS [J]	1 <sup>[1,2]</sup>		
FS [N]	60 <sup>[1]</sup> , less sensitive than LA <sup>[1]</sup> , 60 (100–500 µm grain size) <sup>[2]</sup>		
ESD [J]	200 mJ <sup>[1]</sup> , less sensitive than LA <sup>[1]</sup> , 0.2 (100–500 µm grain size) <sup>[2]</sup>		
N [%]	51.85		
Ω(CO <sub>2</sub> ) [%]	-53.3		
T <sub>m.p.</sub> [°C]	240 <sup>[1]</sup>		
T <sub>dec.</sub> [°C]	240 K (onset) <sup>[1]</sup> , 242 (onset, DSC @ 5 °C/min) <sup>[2]</sup>		
ρ [g cm <sup>-3</sup> ]	1.86 <sup>[1]</sup> , 1.864 <sup>[2]</sup>		
Heat of formation	358 kJ/mol (Δ <sub>f</sub> H <sub>m</sub> <sup>0</sup> ) <sup>[2]</sup> , 1417 kJ/kg (Δ <sub>f</sub> U <sup>0</sup> ) <sup>[2]</sup>		
	Calcd. (EXPLO5.4)	Lit. values	Exptl.
-Δ <sub>ex</sub> U <sup>0</sup> [kJ kg <sup>-1</sup> ]	4,747 (@ 1.864 g cm <sup>-3</sup> ) <sup>[2]</sup>		

$T_{\text{ex}}$ [K]	3,450 (@ 1.864 g cm <sup>-3</sup> ) <sup>[2]</sup>		
$p_{\text{CJ}}$ [kbar]	309 (@ 1.864 g cm <sup>-3</sup> ) <sup>[2]</sup>		
VoD [m s <sup>-1</sup> ]	8,511 (@ 1.864 g cm <sup>-3</sup> ) <sup>[2]</sup>	8,500 (@ 1.86 g cm <sup>-3</sup> ) <sup>[1]</sup>	
$V_0$ [L kg <sup>-1</sup> ]	702 (@ 1.864 g cm <sup>-3</sup> ) <sup>[2]</sup>		
Thermal stability	>200 °C <sup>[1]</sup>		

	DNBTM <sup>[2]</sup>
Chemical formula	C <sub>5</sub> H <sub>6</sub> N <sub>10</sub> O <sub>4</sub>
Molecular weight [g mol <sup>-1</sup> ]	270.2
Crystal system	Monoclinic
Space group	P2 <sub>1</sub> /n
$a$ [Å]	8.356(2)
$b$ [Å]	4.914 (1)
$c$ [Å]	23.689(2)
$\alpha$ [°]	90
$\beta$ [°]	98.232(7)
$\gamma$ [°]	90
$V$ [Å <sup>3</sup> ]	962.77(12)
$Z$	4
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.864
$T$ [K]	173

[1] S. R. Ahmad, M. Cartwright, *Laser Ignition of Energetic Materials*, Wiley, 2015.

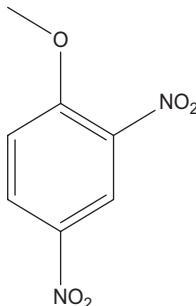
[2] A. A. Dippold, M. Feller, T. M. Klapötke, *Centr. Eur. J. Energet. Mater.*, 2011, 8, 261–278.

## 2,4-Dinitroanisole

Name [German, acronym]: 2,4-Dinitroanisole, 1-methoxy-2,4-dinitrobenzene, 2,2-dinitrophenyl methyl ether, 2,4-dinitro-1-methoxybenzene [2,4-dinitroanisol, DNAN, 2,4-DNAs]\*

Main (potential) use: TNT replacement in melt-cast formulations<sup>[1,18,20,23]</sup>, for example in PAX explosives<sup>[8,23]</sup>, in several US fills such as mortar high explosive fragmentation charges<sup>[18]</sup> and in the SPIDER defense system<sup>[18]</sup>, was used in warheads<sup>[23]</sup>, used in the WW-II as component of Amatol 40<sup>[23]</sup>, ingredient in low-sensitivity melt-cast formulations<sup>[23]</sup>

Structural formula:



\*Two stable isomers of dinitroanisole have been isolated, namely, 2,4-dinitroanisole and 2,6-dinitroanisole, but only 2,4-dinitroanisole shows explosive properties<sup>[23]</sup>.

	<b>DNAN</b>
Formula	C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> O <sub>5</sub>
Molecular mass [g mol <sup>-1</sup> ]	198.13
Appearance at RT	Crystalline substance <sup>[26]</sup>
IS [J]	>50 <sup>[2]</sup> , Rotter FOI >220 <sup>[7]</sup> , H <sub>50%</sub> ≥ 100 cm (ARDEC ERL apparatus, 2.5 kg mass, type 12 tool) <sup>[8]</sup> , H <sub>50</sub> = 117.5 cm (5 kg mass) <sup>[20]</sup> , >24 (BAM) <sup>[21]</sup>
FS [N]	170 <sup>[1]</sup> , >360 <sup>[2]</sup> , 160 (Julius-Peters BAM friction tester) <sup>[7]</sup> , 128 (some reactions, BAM) <sup>[8]</sup> , no reactions @ 120 (BAM) <sup>[8]</sup> , 160 <sup>[19]</sup> , 160 (Julius-Peters apparatus) <sup>[21]</sup>
ESD [J]	4.5 (ignition) <sup>[7]</sup> , 4.5 (Nexter Munitions apparatus) <sup>[21]</sup>
N [%]	14.14

$\Omega(\text{CO}_2)$ [%]	-96.9		
$T_{\text{m.p.}}$ [°C]	94.5 <sup>[2,3,9]</sup> , 97.2 (DSC) <sup>[7]</sup> , 93.92 (onset, DSC @ 5 °C/min) <sup>[8]</sup> , 92–96 <sup>[8]</sup> , ~ 89 (technical grade) <sup>[11]</sup> , 86.9 (labile form) <sup>[11]</sup> , 94.6 (stable form) <sup>[11]</sup> , 95 (form I, Nyburg) <sup>[12]</sup> , 87 (form II, Xue) <sup>[12]</sup> , 94–95 <sup>[18]</sup> , 95 <sup>[19]</sup> , 367 K <sup>[20]</sup> , 92 <sup>[21]</sup> , 367.65 K <sup>[23]</sup> , 359.9 K <sup>[23]</sup> , freezing points: 86.9 (modification I) and 95 (modification II) <sup>[26]</sup> , 359.9 K <sup>[28]</sup> , 88 <sup>[29]</sup>		
$T_{\text{b.p.}}$ [°C]	479.15 K (@ 12 mm Hg) <sup>[23]</sup> , 588 K <sup>[23]</sup> , 592.77 K <sup>[23]</sup> , 587.6 K ( $T_{\text{nbp}}$ , est. Stein-Brown method) <sup>[28]</sup>		
$T_{\text{phase transition}}$ [°C]	$\beta$ - shows phase transition on cooling @ 264.5 K <sup>[14]</sup>		
$T_{\text{dec.}}$ [°C]	261.93 <sup>[4]</sup> , 226.13 (onset, DSC @ 5 °C/min) <sup>[8]</sup>		
$\rho$ [g cm <sup>-3</sup> ]	1.546 <sup>[2,27]</sup> , 1.444 ± 0.06 (@ 293.15 K) <sup>[5]</sup> , 1.52 <sup>[8]</sup> , 1.336 (crystal) <sup>[9]</sup> , 1.341 (@ 20 °C, technical grade) <sup>[11]</sup> , 1.336 <sup>[20]</sup>		
Heat of formation	−186.65 kJ/mol (enthalpy of form.) <sup>[2,27]</sup> , −942.03 kJ/kg (enthalpy of form.) <sup>[2]</sup> , 45.0 kcal/mol ( $Q_f^{\text{P}}$ ) <sup>[11]</sup> , −44 kcal/mol <sup>[20]</sup> , 198.5 kcal/kg <sup>[25]</sup> , 46.42 kcal/mol <sup>[26]</sup> , −186.6 ± 3.4 kJ/mol ( $\Delta H_f^{\circ}$ , (c)) <sup>[30]</sup>		
Heat of combustion	$Q_c^{\text{V}} = 4145.7$ kcal/kg <sup>[25]</sup> , $Q_c^{\text{P}} = 820.2$ kcal/mol <sup>[11]</sup>		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^{\circ}$ [kJ kg <sup>-1</sup> ]	3,692	92.1 kcal/mol ( $Q_e$ ) <sup>[11]</sup>	
$T_{\text{ex}}$ [K]	2,743	2,455 (@ 1.546 g cm <sup>-3</sup> , $\Delta H_f = -186.5$ kJ/mol, calcd., JAGUAR) <sup>[27]</sup>	
$p_{\text{C-J}}$ [kbar]	159	119 (@ 1.341 g cm <sup>-3</sup> , calcd., K-J) <sup>[6]</sup>  9.51 GPa (calcd., CHEETAH v2.0) <sup>[7]</sup>  13.3 GPa (@ 1.546 g cm <sup>-3</sup> , calcd., CHEETAH 1998) <sup>[10]</sup>  16.6 GPa (@ 1.56 g cm <sup>-3</sup> , calcd., CHEETAH 3) <sup>[19]</sup>  13.3 GPa (@ 1.546 g cm <sup>-3</sup> , $\Delta H_f^{\circ} = -186.6$ kJ/mol, calcd., CHEETAH) <sup>[22]</sup>	

		14.8 GPa (@ 1.546 g cm <sup>-3</sup> , $\Delta H_f = -186.5 \text{ kJ/mol}$ , calcd., JAGUAR) <sup>[27]</sup>	
VoD [m s <sup>-1</sup> ]	6,241 (@ 1.556 g cm <sup>-3</sup> , $\Delta_f H = -186.65 \text{ kJ}$ mol <sup>-1</sup> )	5,706 (@ 1.341 g cm <sup>-3</sup> , calcd., K-J) <sup>[6]</sup>  5,344 (calcd. CHEETAH v2.0) <sup>[7]</sup>  6,000 (@ 1.546 g cm <sup>-3</sup> , calcd., CHEETAH 1998) <sup>[10]</sup>  6,742 (@ 1.56 g cm <sup>-3</sup> , calcd., CHEETAH 3) <sup>[19]</sup>  6,000 (@ 1.546 g cm <sup>-3</sup> , $\Delta H_f^\circ = -186.6 \text{ kJ/mol}$ , calcd., CHEETAH) <sup>[22]</sup>  6,140 (@ 1.546 g cm <sup>-3</sup> , $\Delta H_f = -186.5 \text{ kJ/mol}$ , calcd., JAGUAR) <sup>[27]</sup>  6,070 (@ 1.52 g cm <sup>-3</sup> , calcd., JAGUAR) <sup>[27]</sup>  5,890 (@ 1.45 g cm <sup>-3</sup> , calcd., JAGUAR) <sup>[27]</sup>	5,670 <sup>[8]</sup>  5,590 (casted) <sup>[8]</sup>  5,320 (@ 1.34 g cm <sup>-3</sup> ) <sup>[21]</sup>  5,960 (@ 1.52 g cm <sup>-3</sup> ) <sup>[27]</sup>  5,690 (@ 1.45 g cm <sup>-3</sup> ) <sup>[27]</sup>
$V_0$ [L kg <sup>-1</sup> ]	626		726 <sup>[26]</sup>

Critical temperature [°C]	806 K <sup>[23]</sup> , 806.3 K (est. Joback-Stein method) <sup>[28]</sup> , 938.9 K (est. Valderrama-Alveraz method) <sup>[28]</sup>
Critical pressure	39.9 bar <sup>[23]</sup> , 39.9 bar (est. Joback-Stein method) <sup>[28]</sup> , 34.67 bar (est. Valderrama-Alveraz method) <sup>[28]</sup>
Ballistic mortar test	87% TNT <sup>[13]</sup>
LSGT [cm]	71 cards (50% card gap, 70.2 kbars, 0.709 in) <sup>[8]</sup>
5 s explosion $T$ [°C] Ignition $T$ [°C] Initiation $T$ [°C]	347 <sup>[7,23]</sup> 347 <sup>[21]</sup>
Flash point [°C]	180.5 ± 24.3 <sup>[23]</sup>

Vacuum stability test [cm <sup>3</sup> /h]	<0.5 mL/g (5 g sample, 100 °C, 48 h) <sup>[8]</sup>																			
Vapor pressure [atm @ °C]	0.000145 mm Hg <sup>[23]</sup> , 0.000138 mm Hg @ 25 °C <sup>[23]</sup> , 8.95 × 10 <sup>-5</sup> Torr @ 298.15 K <sup>[23]</sup>  Calcd. vapor pressure (ChemCad model, approx. values); vapor pressure (psi)/T(°C) <sup>[23]</sup> : 2/30, 4/40, 4/50, 20/80, 38/100, 62/120, 85/130, 115/140, 145/150 <sup>[23]</sup>																			
Viscosity	5.05 mPa s (@ 373 K) <sup>[20]</sup>																			
Solubility [g/mL]	0.14 g/L in H <sub>2</sub> O @ 298.15 K <sup>[23]</sup> , 0.159 g/L in H <sub>2</sub> O @ 298.15 K <sup>[23]</sup> , 276.2 mg/L in H <sub>2</sub> O @ 25 °C <sup>[24]</sup> , 213 mg/L in H <sub>2</sub> O @ 25 °C <sup>[24]</sup> , 1.550E-01 g/L in H <sub>2</sub> O @ 15 °C <sup>[29]</sup> , 1.360E-01 g/L in H <sub>2</sub> O @ 50 °C <sup>[29]</sup> , 4.757E+00 g/l in H <sub>2</sub> O @ 100 °C <sup>[29]</sup>  Aqueous solubility of DNAN in the presence of NaCl or CaCl <sub>2</sub> <sup>[23]</sup> :  <table border="1"> <thead> <tr> <th rowspan="2">Vol. % salt soln.</th><th colspan="3">Temperature (K)</th></tr> <tr> <th>298.15</th><th>308.15</th><th>318.15</th></tr> </thead> <tbody> <tr> <td>0</td><td>276.2 ± 2.5</td><td>399.2 ± 4.0</td><td>560.0 ± 5.0</td></tr> <tr> <td>1% NaCl</td><td>267.1 ± 2.5</td><td>388.6 ± 3.0</td><td>527.2 ± 5.0</td></tr> <tr> <td>1% CaCl<sub>2</sub></td><td>268.1 ± 2.5</td><td>388.8 ± 3.0</td><td>537.5 ± 5.0</td></tr> </tbody> </table>	Vol. % salt soln.	Temperature (K)			298.15	308.15	318.15	0	276.2 ± 2.5	399.2 ± 4.0	560.0 ± 5.0	1% NaCl	267.1 ± 2.5	388.6 ± 3.0	527.2 ± 5.0	1% CaCl <sub>2</sub>	268.1 ± 2.5	388.8 ± 3.0	537.5 ± 5.0
Vol. % salt soln.	Temperature (K)																			
	298.15	308.15	318.15																	
0	276.2 ± 2.5	399.2 ± 4.0	560.0 ± 5.0																	
1% NaCl	267.1 ± 2.5	388.6 ± 3.0	527.2 ± 5.0																	
1% CaCl <sub>2</sub>	268.1 ± 2.5	388.8 ± 3.0	537.5 ± 5.0																	
	Dissolves in water with difficulty <sup>[26]</sup> , more soluble in EtOH and Et <sub>2</sub> O <sup>[26]</sup> , very soluble in acetone and benzene <sup>[26]</sup> , 0.276 g/L H <sub>2</sub> O <sup>[28]</sup>																			
Log K <sub>ow</sub>	1.612 ± 0.014 @ 298.15 K <sup>[23]</sup> , 1.549 ± 0.013 @ 308.15 K <sup>[23]</sup> , 1.472 ± 0.025 @ 318.15 K <sup>[23]</sup> , 1.58 <sup>[24]</sup> , 1.64 <sup>[24]</sup> , 1.70–1.92 <sup>[24]</sup> , 1.612 (@ 298.15 K) <sup>[28]</sup> , 2.38 (est., Broto method) <sup>[28]</sup> , 1.70 (est., Ghose) <sup>[28]</sup> , 1.92 (est., COSMOTHERM) <sup>[28]</sup>																			
Log K <sub>oc</sub>	2.2 <sup>[24]</sup>																			
Enthalpy of fusion [kJ/mol]	19.91 <sup>[23]</sup> , 19.91 (est.) <sup>[26]</sup>																			
Enthalpy of vaporization [kJ/mol]	57.21 ± 3.0 @ 298.15 K <sup>[23]</sup>																			
Dipole moment [Debye]	3.83 <sup>[23]</sup>																			
Biodegradation	Complete aerobic transformation in 34 days in soils and slurries supplemented with carbon and nitrogen sources <sup>[23]</sup> , complete biotransformation in 8 days in soils by <i>Bacillus</i> Sp. <sup>[23]</sup>																			
Fugacity	245 cc <sup>[26]</sup>																			

	2,4-Dinitroanisole <sup>[15,23]</sup>	2,4-Dinitroanisole <sup>[14]</sup>	2,4-Dinitroanisole <sup>[14]</sup>	2,4-Dinitroanisole <sup>[14]</sup>	2,4-Dinitroanisole <sup>[14]</sup>
Chemical formula	C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> O <sub>5</sub>	C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> O <sub>5</sub>	C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> O <sub>5</sub>	C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> O <sub>5</sub>	C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> O <sub>5</sub>
Molecular weight [g mol <sup>-1</sup> ]	198.13	198.14	198.14	198.14	198.14
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	P <sub>2</sub> <sub>1</sub> /n (no. 14)				
<i>a</i> [Å]	8.772(2)	3.957(2)	3.9291(18)	3.908(2)	3.8968(16)
<i>b</i> [Å]	12.645(2)	13.735(7)	13.739(6)	13.78(1)	13.781(7)
<i>c</i> [Å]	15.429(4)	15.454(8)	15.443(7)	15.42(1)	15.419(7)
$\alpha$ [ $^{\circ}$ ]	90	90	90	90	90
$\beta$ [ $^{\circ}$ ]	81.89(2)	91.156(8)	94.454(7)	95.310(6)	95.382(6)
$\gamma$ [ $^{\circ}$ ]	90	90	90	90	90
<i>V</i> [Å <sup>3</sup> ]	1694	839.7(7)	831.1(6)	826.8(9)	824.4(7)
<i>Z</i>	8	4	4	4	4
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.56	1.567	1.583	1.592	1.596
<i>T</i> [K]	298	273	261	236	226

2,4-Dinitroanisole has two polymorphic structures:  $\alpha$ - and  $\beta$ -<sup>[14]</sup>

	2,4-Dinitroanisole <sup>[16]</sup>	2,4-Dinitroanisole <sup>[17]</sup>	2,4-Dinitroanisole <sup>[14]</sup>	2,4-Dinitroanisole <sup>[14]</sup>	2,4-Dinitroanisole <sup>[14]</sup>
Chemical formula	C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> O <sub>5</sub>	C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> O <sub>5</sub>	C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> O <sub>5</sub>	C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> O <sub>5</sub>	C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> O <sub>5</sub>
Molecular weight [g mol <sup>-1</sup> ]	198.13	198.13	198.13	198.13	198.13
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	P <sub>2</sub> <sub>1</sub> /n (no. 14)				
<i>a</i> [Å]	15.488(6)	3.9793(9)	3.980(2)	3.9618(19)	3.880(2)

<i>b</i> [Å]	8.813(3)	13.7592(11)	13.759(7)	13.745(7)	13.786(7)
<i>c</i> [Å]	12.699(4)	15.4453(14)	15.461(8)	15.470(8)	15.404(9)
$\alpha$ [°]	90	90	90	90	90
$\beta$ [°]	90	90.887(11)	90.994(8)	91.089(6)	95.639(7)
$\gamma$ [°]	82.06(3)	90	90	90	90
<i>V</i> [Å <sup>3</sup> ]	1716.74	845.6(2)	846.5(7)	842.3(79)	820.0(8)
<i>Z</i>	8	4	4	4	4
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.533	1.556	1.555	1.563	1.605
<i>T</i> [K]	295	293	298	283	208

	2,4-Dinitroanisole <sup>[14]</sup>	2,4-Dinitroanisole <sup>[14]</sup>	2,4-Dinitroanisole <sup>[14]</sup>	2,4-Dinitroanisole <sup>[14]</sup>
Chemical formula	C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> O <sub>5</sub>	C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> O <sub>5</sub>	C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> O <sub>5</sub>	C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> O <sub>5</sub>
Molecular weight [g mol <sup>-1</sup> ]	198.13	198.13	198.13	198.13
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	<i>P</i> 2 <sub>1</sub> /n (no. 14)			
<i>a</i> [Å]	3.8760(18)	3.8537(15)	3.8278(18)	3.8139(10)
<i>b</i> [Å]	13.791(6)	13.804(5)	13.813(6)	13.823(4)
<i>c</i> [Å]	15.388(7)	15.381(6)	15.364(8)	15.349(4)
$\alpha$ [°]	90	90	90	90
$\beta$ [°]	95.882(6)	96.164(6)	96.512(7)	96.777(4)
$\gamma$ [°]	90	90	90	90
<i>V</i> [Å <sup>3</sup> ]	818.2(6)	813.5	807.1(7)	803.5(4)
<i>Z</i>	4	4	4	4
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.608	1.618	1.631	1.638
<i>T</i> [K]	198	173	128	100

Neutron powder diffraction results at different temperatures and pressures<sup>[12]</sup>:

DNAN form	T (K)	p (GPa)	a (Å)	b (Å)	c (Å)	β (°)	V (Å <sup>3</sup> )
II	295	0.0001	3.9767(1)	13.7441(7)	15.4547(6)	91.067(4)	844.54(4)
III	100	0.0001	3.80708(7)	13.8042(3)	15.3387(3)	96.742(2)	800.53(2)
II	295	0.01	3.9573(6)	13.720(4)	15.426(3)	91.11(2)	837.3(2)
III	295	0.16	3.8821(4)	13.717(2)	15.402(2)	94.32(2)	817.8(2)
III	295	0.53	3.7827(2)	13.710(1)	15.293(1)	95.693(8)	789.20(9)
III	295	1.11	3.6801(2)	13.679(1)	15.177(1)	96.647(8)	758.90(7)
III	295	2.02	3.5658(2)	13.622(1)	15.044(1)	97.536(8)	724.4(7)
III	295	2.88	3.4940(2)	13.572(1)	14.956(1)	98.013(7)	702.30(6)

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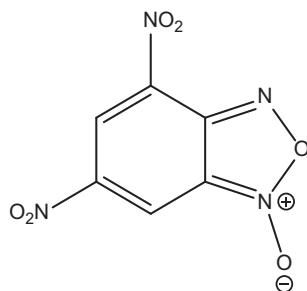
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## 4,6-Dinitrobenzofuroxan

Name [German, acronym]: 4,6-Dinitrobenzofuroxan, 4,6-dinitrobenzofurazan-1-oxide, dinitro-dinitrosobenzene  
[4,6-Dinitrobenzofuroxan, 4,6-DNBF]

Main (potential) use: Key intermediate in the synthesis of many primary explosives which are being investigated for possible applications<sup>[10]</sup>

Structural formula:



	<b>4,6-Dinitrobenzofuroxan</b>
Formula	C <sub>6</sub> H <sub>2</sub> N <sub>4</sub> O <sub>6</sub>
Molecular mass [g mol <sup>-1</sup> ]	226.10
Appearance at RT	
IS [J]	Rotter impact F of I is 89 (cf. RDX = 80), 100% height 170 cm, 0% height 90 cm, 5 kg mass <sup>[3]</sup> , log H <sub>50%</sub> = 1.48 <sup>[5]</sup> , H <sub>50%</sub> = 76 cm (B.M., type 12 tool, 2.5 kg mass, 35 mg sample, garnet paper) <sup>[7]</sup> , H <sub>50%</sub> = 76 cm (19 J) <sup>[11]</sup> , H <sub>50%</sub> = 76 cm (2.5 kg mass, type 12 tool) <sup>[13]</sup> , H <sub>50%</sub> = 76 cm (2.5 kg mass, type 12 tool, 35 mg sample in conical pile, 1 in <sup>2</sup> garnet paper) <sup>[16]</sup> , H <sub>50%</sub> = 76 cm (2.5 kg mass) <sup>[17]</sup>
FS [N]	Ignites at 4.5 J but not at 0.45 J <sup>[3]</sup>
N [%]	24.78
Ω(CO <sub>2</sub> ) [%]	-49.5
T <sub>m.p.</sub> [°C]	172 <sup>[1,3,8]</sup> , 174 (DTA @ 10 K/min, 10 mg sample) <sup>[6]</sup> , 173–174 <sup>[15]</sup> , 174 (endo, DTA, 2–3 mg sample @ 10 °C/min, static air) <sup>[15]</sup>
T <sub>dec.</sub> [°C]	~245 (DSC @ 10 °C/min) <sup>[3]</sup> , 273 (DTA @ 10 K/min, 10 mg sample) <sup>[6]</sup> , 273 (exo, DTA 2–3 mg sample, @ 10 °C/min, static air) <sup>[15]</sup>
ρ [g cm <sup>-3</sup> ]	2.21 ± 0.1 (@ 20 °C) <sup>[2]</sup> , 1.76 (ρ <sub>obs.</sub> ) <sup>[16]</sup> , 1.759 (X-ray @ 288 K) <sup>[9]</sup>

Heat of formation	203.0 kcal/kg (enthalpy of form.) <sup>[12]</sup>		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^{\circ}$ [kJ kg <sup>-1</sup> ]		1216 kcal/kg (@ 1.690 g cm <sup>-3</sup> , calcd.) [H <sub>2</sub> O vapor] <sup>[12]</sup>	1160 [H <sub>2</sub> O (g)] <sup>[4]</sup> 1160 kcal/kg (@ 1.690 g cm <sup>-3</sup> ) [H <sub>2</sub> O vapor] <sup>[12]</sup>
$T_{\text{ex}}$ [K]			
$p_{\text{CJ}}$ [GPa]		263 kbar (@ 1.86 g cm <sup>-3</sup> , calcd.) <sup>[16]</sup>	
VoD [m s <sup>-1</sup> ]		7,700 (@ 1.86 g cm <sup>-3</sup> , calcd.) <sup>[16]</sup>	7,480 (@ 96.2 % TMD, 2.025 mm charge diameter) <sup>[14]</sup>  7,325 (@ 96.2 % TMD, 1.52 mm charge diameter) <sup>[14]</sup>  7,522 (@ 96.2 % TMD, 4.05 mm charge diameter) <sup>[14]</sup>  7,616 (@ 94.5 % TMD, 12.75 mm charge diameter) <sup>[14]</sup>  7,535 (@ 94.5 % TMD, 5.95 mm charge diameter) <sup>[14]</sup>  7,578 (@ 94.5 % TMD, 5.95 mm charge diameter) <sup>[14]</sup>  7,458 (@ 94.5 % TMD, 4.05 mm charge diameter) <sup>[14]</sup>  6,786 (@ 94.5 % TMD, 2.025 mm charge diameter) <sup>[14]</sup>

			7,422 (@ 90.4 % TMD, 12.75 mm charge diameter) <sup>[14]</sup>
			7,414 (@ 90.4 % TMD, 5.95 mm charge diameter) <sup>[14]</sup>
			7,449 (@ 90.4 % TMD, 4.05 mm charge diameter) <sup>[14]</sup>
			7,313 (@ 90.4 % TMD, 4.05 mm charge diameter) <sup>[14]</sup>
			7,092 (@ 90.4 % TMD, 2.025 mm charge diameter) <sup>[14]</sup>
$V_0$ [L kg <sup>-1</sup> ]			

Critical diameter [cm]	<1.52 mm @ 96.2% TMD <sup>[10]</sup> , $d_c < 1.5$ mm @ 96.2% TMD <sup>[14]</sup> , $d_c < 2.0$ mm @ 90.4% TMD <sup>[14]</sup>
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	<b>DNBF<sup>[9]</sup></b>
Chemical formula	C <sub>6</sub> H <sub>2</sub> N <sub>4</sub> O <sub>6</sub>
Molecular weight [g mol <sup>-1</sup> ]	226.12
Crystal system	Monoclinic
Space group	P21
<i>a</i> [\AA]	7.408(2)
<i>b</i> [\AA]	6.185(1)
<i>c</i> [\AA]	9.796(2)
$\alpha$ [°]	90
$\beta$ [°]	107.99(2)
$\gamma$ [°]	90
<i>V</i> [\AA <sup>3</sup> ]	426.90(16)
<i>Z</i>	2
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.759
<i>T</i> [K]	288

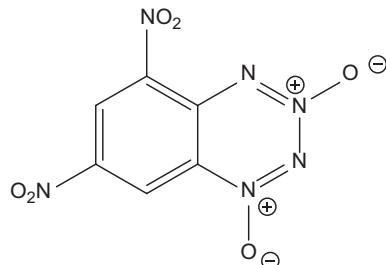
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## 5,7-Dinitrobenzo-1,2,3,4-tetrazine-1,3-dioxide

Name [German, acronym]: 5,7-Dinitrobenzo[1,2,3,4]tetrazine 1,3-dioxide, [DNBTDO, 5,7-DNBTDO]

Main (potential) use: secondary explosive

Structural formula:



	<b>DNBTDO</b>										
Formula	C <sub>6</sub> H <sub>2</sub> N <sub>6</sub> O <sub>6</sub>										
Molecular mass [g mol <sup>-1</sup> ]	254.12										
Appearance at RT	Yellow rod crystals from dichloromethane <sup>[2]</sup>										
IS [J]	<p>4–6 (depends on particle size)<sup>[1]</sup>, 5 (BAM)<sup>[2]</sup></p> <p>IS with different particle sizes, BAM<sup>[2]</sup>:</p> <table border="1"> <thead> <tr> <th>Particle size (µm)</th> <th>IS (J)</th> </tr> </thead> <tbody> <tr> <td>&lt;100</td> <td>6</td> </tr> <tr> <td>100–500</td> <td>5</td> </tr> <tr> <td>500–1,000</td> <td>4</td> </tr> <tr> <td>&gt;1000</td> <td>4</td> </tr> </tbody> </table>	Particle size (µm)	IS (J)	<100	6	100–500	5	500–1,000	4	>1000	4
Particle size (µm)	IS (J)										
<100	6										
100–500	5										
500–1,000	4										
>1000	4										
FS [N]	<p>360<sup>[1]</sup>, 360 (BAM)<sup>[2]</sup></p> <p>FS with different particle sizes, BAM<sup>[2]</sup>:</p> <table border="1"> <thead> <tr> <th>Particle size (µm)</th> <th>FS (N)</th> </tr> </thead> <tbody> <tr> <td>&lt;100</td> <td>360</td> </tr> <tr> <td>100–500</td> <td>360</td> </tr> <tr> <td>500–1,000</td> <td>360</td> </tr> <tr> <td>&gt;1,000</td> <td>360</td> </tr> </tbody> </table>	Particle size (µm)	FS (N)	<100	360	100–500	360	500–1,000	360	>1,000	360
Particle size (µm)	FS (N)										
<100	360										
100–500	360										
500–1,000	360										
>1,000	360										
ESD [J]	0.15 <sup>[1]</sup> , 0.15 (100–500 µm particle size, ESD 2010EN, OZM research) <sup>[2]</sup>										
N [%]	33.07										

$\Omega(\text{CO}_2)$ [%]	-44.1		
$T_{\text{m.p.}}$ [°C]	204 (dec., DSC @ 5 °C/min) <sup>[2]</sup> , no melting before dec. observed <sup>[2]</sup>		
$T_{\text{dec.}}$ [°C]	483 K (onset) <sup>[1]</sup> , 204 (onset, dec., DSC @ 5 K/min) <sup>[2]</sup> , 211.8 (onset) <sup>[2]</sup>		
$\rho$ [g cm <sup>-3</sup> ]	1.868 (single crystal @ 173 K, X-ray) <sup>[2]</sup>		
Heat of formation	420 kJ/mol ( $\Delta H_f^\circ$ , solid state energy of form., bomb calorimetry, Hess' law) <sup>[2]</sup> , 475.3 kJ/mol ( $\Delta H_f(s)$ ) <sup>[2]</sup> , 442.7 kJ/mol ( $\Delta U_f(s)$ ) <sup>[2]</sup>		
Heat of combustion	14,846 kJ/g (exptl. Parr bomb calorimeter) <sup>[2]</sup>		
	Calcd. (EXPLO5 5.04)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^\circ$ [kJ kg <sup>-1</sup> ]	6,306.7 ( $Q^\circ$ @ 1.868 g/cm <sup>3</sup> ) <sup>[2]</sup>		
$T_{\text{ex}}$ [K]	4,659 (@ 1.868 g/cm <sup>3</sup> ) <sup>[2]</sup>		
$p_{\text{CJ}}$ [kbar]	33.0 GPa (@ 1.868 g/cm <sup>3</sup> ) <sup>[2]</sup>		
VoD [m s <sup>-1</sup> ]	8,411 (@ 1.868 g/cm <sup>3</sup> ) <sup>[2]</sup>		
$V_0$ [L kg <sup>-1</sup> ]	576 (@ 1.868 g/cm <sup>3</sup> ) <sup>[2]</sup>		
Solubility [g/mL]	Recryst. from dichloromethane <sup>[2]</sup> , soluble in acetone <sup>[2]</sup>		
Heat of subl. [kJ/mol]	77.9 (Troutman rule) <sup>[2]</sup>		
SSRT	Sample weight = 505 mg, dent = 744 mg SiO <sub>2</sub> <sup>[2]</sup>		

	DNBTDO <sup>[2]</sup>
Chemical formula	C <sub>6</sub> H <sub>2</sub> N <sub>6</sub> O <sub>6</sub>
Molecular weight [g mol <sup>-1</sup> ]	254.14
Crystal system	Orthorhombic
Space group	Pca2 <sub>1</sub> (no. 29)
$a$ [\AA]	9.8893(15)
$b$ [\AA]	17.859(3)
$c$ [\AA]	10.2341(13)
$\alpha$ [°]	90
$\beta$ [°]	90
$\gamma$ [°]	90
$V$ [\AA <sup>3</sup> ]	1,807.5(5)

Z	8
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.868
T [K]	173

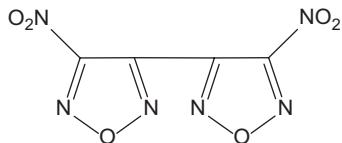
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## 4,4'-Dinitro-3,3'-bifurazan

Name [German, acronym]: Dinitrobifurazan, DNBF

Main (potential) use: Possible future ingredient for high-performance castable explosives<sup>[1]</sup>

Structural formula:



	DNBF															
Formula	$C_4N_6O_6$															
Molecular mass [g mol <sup>-1</sup> ]	228.08															
Appearance at RT																
IS [J]	12 cm <sup>[1]</sup>  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 ref. <sup>[2]</sup> <table border="1" style="margin-left: auto; margin-right: auto;"> <thead> <tr> <th colspan="2">Rotter impact data</th> <th colspan="2">US data</th> </tr> <tr> <th>F of I</th> <th>Gas evolved (mL)</th> <th>NSWC/NOL, ERL type 12</th> <th>NWC B.M. type 12</th> </tr> </thead> <tbody> <tr> <td>90</td> <td>19.8</td> <td></td> <td>18, 76</td> </tr> </tbody> </table>				Rotter impact data		US data		F of I	Gas evolved (mL)	NSWC/NOL, ERL type 12	NWC B.M. type 12	90	19.8		18, 76
Rotter impact data		US data														
F of I	Gas evolved (mL)	NSWC/NOL, ERL type 12	NWC B.M. type 12													
90	19.8		18, 76													
N [%]	36.85															
$\Omega(CO_2)$ [%]	-14.0															
$T_{m.p.}$ [°C]	85 <sup>[1]</sup>															
$\rho$ [g cm <sup>-3</sup> ]	1.92 (crystal, calcd.) <sup>[1]</sup> , 1.85 (crystal, flotation) <sup>[1]</sup>															
Heat of formation																
	Calcd. (EXPLO5 6.03)		Lit. values	Exptl.												
$-\Delta_{ex}U^\circ$ [kJ kg <sup>-1</sup> ]																
$T_{ex}$ [K]																
$p_{CJ}$ [kbar]			35.6 GPa (calcd.) <sup>[1]</sup>													

VoD [ $\text{m s}^{-1}$ ]		8,800 ( $\rho$ not specified, calcd.) <sup>[1]</sup>	
$V_0$ [ $\text{L kg}^{-1}$ ]			

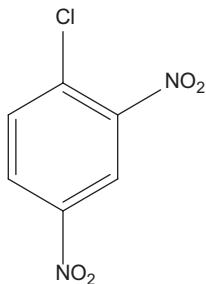
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## Dinitrochlorobenzene

Name [German, acronym]: Dinitrochlorobenzene, 1-chloro-2,4-dinitrobenzene, parazol, 2,4-dinitro-1-chlorobenzene, 4-chloro-1,3-dinitrobenzene, 6-chloro-1,3-dinitrobenzene [1,2,4-chlordinitrobenzol, DNCB]

Main (potential) use: Intermediate in synthesis of explosives<sup>[1,11]</sup>, in past was investigated in mixtures with TNT in H.E. shells, since it did not completely detonate it, acted as a lachrymator<sup>[11]</sup>, constituent of some AN and chlorate explosives<sup>[12]</sup>, component of chlorate explosives<sup>[13]</sup>, used in production of dinitrophenol, trinitroanisole and hexite<sup>[13]</sup>

Structural formula:



	DNCB
Formula	C <sub>6</sub> H <sub>3</sub> N <sub>2</sub> O <sub>4</sub> Cl
Molecular mass [g mol <sup>-1</sup> ]	202.55
Appearance at RT	Yellow crystals <sup>[12,14]</sup>
IS [J]	>50 Nm <sup>[1]</sup>
FS [N]	>353 <sup>[1]</sup>
N [%]	13.83
Ω(CO <sub>2</sub> ) [%]	-71.1
T <sub>m.p.</sub> [°C]	53 <sup>[2]</sup> , 325 K <sup>[5]</sup> , 316 K (supercooling α melt) <sup>[5]</sup> , 50 <sup>[6]</sup> , 53.4 (α-DNCB) <sup>[7]</sup> , 43 (β-DNCB) <sup>[7]</sup> , 27 (γ-DNCB) <sup>[7]</sup> , 53.4 (2,4-DNB) <sup>[11]</sup> , 87–88 (2,6-DNB) <sup>[11]</sup> , 52–54 <sup>[12,14]</sup>
T <sub>b.p.</sub> [°C]	315 <sup>[12,14]</sup>
ρ [g cm <sup>-3</sup> ]	1.697 <sup>[1]</sup> , 1.619 ± 0.06 (@ 20 °C) <sup>[3]</sup> , sp. gr. = 1.69 <sup>[12]</sup> , ~1.7 <sup>[14]</sup>

Heat of formation	−43.1 kJ/mol (enthalpy of form., calcd., emp.) <sup>[4]</sup> , −24.31 kJ/mol (enthalpy of form., exptl.) <sup>[4]</sup> , −120 kJ/kg (enthalpy of form.) <sup>[1]</sup>		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^{\circ} [\text{kJ kg}^{-1}]$			
$T_{\text{ex}} [\text{K}]$			
$p_{\text{C-J}} [\text{GPa}]$			2,016 kg/cm <sup>2</sup> (@ 0.25 g cm <sup>-3</sup> , pressure obtained in manometric bomb) <sup>[10]</sup>
VoD [m s <sup>-1</sup> ]			
$V_0 [\text{L kg}^{-1}]$			

Solubility [g/mL]	Only poorly soluble in sulfuric acid if conc. < 80% <sup>[10]</sup> data from ref. <sup>[10]</sup> <table border="1"> <thead> <tr> <th rowspan="2">Solvent</th><th colspan="3">Solubility (g/100 g solvent)<sup>[10]</sup></th></tr> <tr> <th>@ 15 °C</th><th>@ various <math>T</math> (°C)</th><th>@ 100 °C</th></tr> </thead> <tbody> <tr> <td>H<sub>2</sub>O</td><td>0.0008</td><td>0.041 @ 50</td><td>0.159</td></tr> <tr> <td>MeOH</td><td>11.226</td><td>32.31 @ 32</td><td></td></tr> <tr> <td>EtOH</td><td>8.246</td><td>18.89 @ 32.5</td><td></td></tr> <tr> <td>Et<sub>2</sub>O</td><td>23.517</td><td>128.13 @ 30.5</td><td></td></tr> <tr> <td>Acetone</td><td>261.9</td><td>581.0 @ 30</td><td></td></tr> <tr> <td>Ethyl acetate</td><td>119.4</td><td>287.5 @ 50</td><td></td></tr> <tr> <td>CHCl<sub>3</sub></td><td>102.76</td><td>210.0 @ 32</td><td></td></tr> <tr> <td>CCl<sub>4</sub></td><td>3.851</td><td>28.87 @ 31</td><td></td></tr> <tr> <td>CS<sub>2</sub></td><td>4.212</td><td></td><td></td></tr> <tr> <td>Benzene</td><td>158.43</td><td>359.64 @ 31</td><td></td></tr> <tr> <td>Toluene</td><td>139.89</td><td>282.55 @ 31.5</td><td></td></tr> <tr> <td>Pyridine</td><td>2.633</td><td>20.85 @ 20</td><td></td></tr> </tbody> </table> Practically insoluble in water <sup>[14]</sup> , sparingly soluble in cold EtOH <sup>[14]</sup> , freely soluble in hot EtOH <sup>[14]</sup> , soluble in benzene, Et <sub>2</sub> O, CS <sub>2</sub> <sup>[14]</sup>				Solvent	Solubility (g/100 g solvent) <sup>[10]</sup>			@ 15 °C	@ various $T$ (°C)	@ 100 °C	H <sub>2</sub> O	0.0008	0.041 @ 50	0.159	MeOH	11.226	32.31 @ 32		EtOH	8.246	18.89 @ 32.5		Et <sub>2</sub> O	23.517	128.13 @ 30.5		Acetone	261.9	581.0 @ 30		Ethyl acetate	119.4	287.5 @ 50		CHCl <sub>3</sub>	102.76	210.0 @ 32		CCl <sub>4</sub>	3.851	28.87 @ 31		CS <sub>2</sub>	4.212			Benzene	158.43	359.64 @ 31		Toluene	139.89	282.55 @ 31.5		Pyridine	2.633	20.85 @ 20	
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	Dinitrochlorobenzen <sup>[7]</sup> ( $\alpha$ -polymorph)	Dinitrochlorobenzen <sup>[8]</sup>	Dinitrochlorobenzen <sup>[9]</sup> ( $\alpha$ -polymorph)	Dinitrochlorobenzen <sup>[6]</sup> ( $\alpha$ -polymorph)	Dinitrochlorobenzen <sup>[5]</sup> ( $\alpha$ -polymorph)	Dinitrochlorobenzen <sup>[5]</sup> ( $\beta$ -polymorph)
Chemical formula	$C_6H_3N_2O_4Cl$	$C_6H_3N_2O_4Cl$	$C_6H_3N_2O_4Cl$	$C_6H_3N_2O_4Cl$	$C_6H_3N_2O_4Cl$	$C_6H_3N_2O_4Cl$
Molecular weight [g mol <sup>-1</sup> ]	202.55	202.55	202.55	202.55	202.55	202.55
Crystal system	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic	Monoclinic
Space group	$Pccn$ (no. 56)	$Pccn$ (no. 56)	$Pccn$ (no. 56)	$Pccn$ (no. 56)	$Pccn$ (no. 56)	$P2_1/c$ (no. 14)
$a$ [Å]	8.937	8.7346(12)	8.939(1)	8.930(1)	8.937(5)	8.91(1)
$b$ [Å]	11.035	10.9404(4)	11.039(1)	11.045(2)	11.035(5)	6.870(5)
$c$ [Å]	15.675	15.6406(5)	15.692(1)	15.676(2)	15.844(5)	12.98(1)
$\alpha$ [°]	90	90	90	90	90	90
$\beta$ [°]	90	90	90	90	90	96.15(5)
$\gamma$ [°]	90	90	90	90	90	90
$V$ [Å <sup>3</sup> ]	1,545.87	1,494.62	1,548.45	1,546.15	1,562.53	789.955
$Z$	8	8	8	8	8	4
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.741	1.8	1.738	1.74	1.722	1.703
$T$ [K]	295	110	295	295	295	295

There are three crystalline forms known: (i)  $\alpha$ -DNCB (stable, recrystallized from conc. nitric acid or EtOH), (ii)  $\beta$ -DNCB (unstable, precipitated from fuming nitric acid on addition of H<sub>2</sub>O, or rapid cooling of molten DNCB) and (iii)  $\gamma$ -DNCB.<sup>[7,11]</sup>

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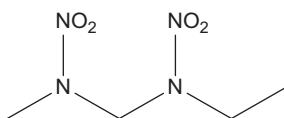
## 2,4-Dinitro-2,4-diazahexane

Name [German, acronym]: 2,4-Dinitro-2,4-diazahexane

[2,4-dinitro-2,4-diazahexan, DNDA-6]

Main (potential) use: Component of DNDA-57 which is used as energetic plasticizer in propellant formulations<sup>[1]</sup>

Structural formula:



	DNDA-6	
Formula	C <sub>4</sub> H <sub>10</sub> N <sub>4</sub> O <sub>4</sub>	
Molecular mass [g mol <sup>-1</sup> ]	178.15	
Appearance at RT		
N [%]	31.45	
Ω(CO <sub>2</sub> ) [%]	-80.83	
T <sub>m,p.</sub> [°C]	33 <sup>[1]</sup> , 31.6 <sup>[2,4,5]</sup>	
T <sub>glass transition</sub> [°C]	-58.3 <sup>[4]</sup>	
T <sub>dec.</sub> [°C]		
ρ [g cm <sup>-3</sup> ]	1.323 ± 0.06 (@ 293.15 K) <sup>[3]</sup> , 1.419 <sup>[4]</sup>	
Heat of formation	-79.5 kJ/mol (Δ <sub>f</sub> H <sup>o</sup> ) <sup>[1]</sup> , -446.24 kJ kg <sup>-1</sup> (Δ <sub>f</sub> H <sup>o</sup> ) <sup>[1]</sup>	
	Calcd. (EXPLO5 6.03)	Exptl.
-Δ <sub>ex</sub> U <sup>o</sup> [kJ kg <sup>-1</sup> ]	4,447	
T <sub>ex</sub> [K]	2,882	
p <sub>C-J</sub> [GPa]	16.43	
VoD [m s <sup>-1</sup> ]	6,840 (@ 1.323 g cm <sup>-3</sup> )	
V <sub>0</sub> [L kg <sup>-1</sup> ]	904	

Melting enthalpy [J/g]	108.2 <sup>[5]</sup>
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	<b>DNDA-6<sup>[4]</sup></b>
Chemical formula	C <sub>4</sub> H <sub>10</sub> N <sub>4</sub> O <sub>4</sub>
Molecular weight [g mol <sup>-1</sup> ]	178.16
Crystal system	Monoclinic
Space group	P2 <sub>1</sub> /c (no. 14)
a [Å]	8.076(5)
b [Å]	10.827(5)
c [Å]	9.528(5)
α [°]	90
β [°]	101.27(1)
γ [°]	90
V [Å <sup>3</sup> ]	817.0(8)
Z	4
ρ <sub>calc</sub> [g cm <sup>-3</sup> ]	1.448
T [K]	183

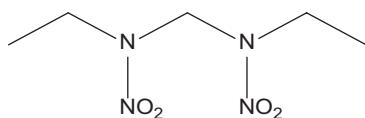
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- [3] Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994–2017 ACD/Labs).
- [4] D. Spitzer, B. Wanders, M. R. Schäfer, R. Welter, *J. Mol. Struct.*, **2003**, *644*, 37–48.
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## 3,5-Dinitro-3,5-diazaheptane

Name [German, acronym]: 3,5-Dinitro-3,5-diazaheptane [3,5-dinitro-3,5-diazaheptan, DNDA-7]

Main (potential) use: Component of DNDA-57 which is used as energetic plasticizer in propellant formulations<sup>[1]</sup>

Structural formula:



	DNDA-7		
Formula	$C_5H_{12}N_4O_4$		
Molecular mass [g mol <sup>-1</sup> ]	192.18		
Appearance at RT			
ESD [J]	12.49 <sup>[5]</sup> , 225.0 mJ <sup>[5]</sup>		
N [%]	29.15		
$\Omega(CO_2)$ [%]	-99.91		
$T_{m.p.}$ [°C]	75 <sup>[1,2,7,8]</sup>		
$T_{\text{glass transition}}$ [°C]	-10.1 <sup>[7]</sup>		
$\rho$ [g cm <sup>-3</sup> ]	1.271 ± 0.06 (@ 20 °C) <sup>[3]</sup> , 1.384 <sup>[6]</sup>		
Heat of formation	-135 kJ/mol ( $\Delta_f H^\circ$ ) <sup>[4]</sup> , -702 kJ kg <sup>-1</sup> ( $\Delta_f H^\circ$ ) <sup>[4]</sup> , -703.01 kJ kg <sup>-1</sup> ( $\Delta_f H^\circ$ ) <sup>[1]</sup>		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^\circ$ [kJ kg <sup>-1</sup> ]	4,081	2,130 (calcd., K-J) <sup>[4]</sup>	
$T_{\text{ex}}$ [K]	2,627		1,425 <sup>[4]</sup>
$p_{\text{CJ}}$ [GPa]	15.45		
VoD [m s <sup>-1</sup> ]	6,730 (@ 1.271 g cm <sup>-3</sup> )		
$V_0$ [L kg <sup>-1</sup> ]	890		
Melting enthalpy [J/g]	163.8 <sup>[8]</sup>		

	<b>DNDA-7<sup>[6]</sup></b>
Chemical formula	C <sub>5</sub> H <sub>12</sub> N <sub>4</sub> O <sub>4</sub>
Molecular weight [g mol <sup>-1</sup> ]	192.19
Crystal system	Monoclinic
Space group	P2 <sub>1</sub> /c (no. 14)
a [Å]	8.531(5)
b [Å]	5.774(5)
c [Å]	18.500(5)
α [°]	90
β [°]	100.821(5)
γ [°]	90
V [Å <sup>3</sup> ]	895.1(10)
Z	4
ρ <sub>calc</sub> [g cm <sup>-3</sup> ]	1.426
T [K]	183

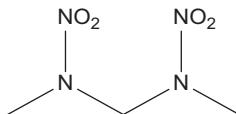
- [1] R. Meyer, J. Köhler, A. Homburg, *Explosives*, 7th edn., Wiley-VCH, Weinheim, **2016**, pp. 103–104.
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## **2,4-Dinitro-2,4-diazapentane**

Name [German, acronym]: 2,4-Dinitro-2,4-diazapentane [2,4-dinitro-2,4-diazapentan, DNDA-5, OCPX, DNAP]

Main (potential) use: Component of DNDA-57 which is used as energetic plasticizer in propellant formulations<sup>[1]</sup>

Structural formula:



	DNDA-5		
Formula	C <sub>3</sub> H <sub>8</sub> N <sub>4</sub> O <sub>4</sub>		
Molecular mass [g mol <sup>-1</sup> ]	164.12		
Appearance at RT			
IS [J]	10 kg, 25 cm = 12% <sup>[8]</sup> , drop energy required for 50% initiation probability ≥ 29.43 (Julius-Peters apparatus, 25 mg sample) <sup>[7]</sup>		
FS [N]	>500 MPa <sup>[8]</sup>		
ESD [J]	13.45 <sup>[5]</sup>		
N [%]	34.14		
Ω(CO <sub>2</sub> ) [%]	-58.49		
T <sub>m,p.</sub> [°C]	54 <sup>[1,8]</sup> , 56 <sup>[2]</sup> , 54.4 (onset) <sup>[6]</sup> , 52–54 <sup>[9]</sup> , 54–57 <sup>[10]</sup> , 54.4 <sup>[11]</sup>		
T <sub>dec.</sub> [°C]	230 <sup>[8]</sup>		
T <sub>glass transition</sub> [°C]	-44.4 <sup>[6]</sup>		
ρ [g cm <sup>-3</sup> ]	1.389 <sup>[1]</sup> , 1.389 ± 0.06 (@ 20 °C) <sup>[3]</sup> , 1.498 <sup>[6]</sup> , 1.50 (calc.) <sup>[8]</sup> , 1.48 <sup>[10]</sup>		
Heat of formation	-51.5 kJ/mol ( $\Delta_f H^\circ$ ) <sup>[4]</sup> , -56.4 ( $\Delta_f H^\circ$ ) kJ/mol <sup>[8]</sup> , -313.8 kJ kg <sup>-1</sup> ( $\Delta_f H^\circ$ ) <sup>[4]</sup> , -314.33 kJ/kg (enthalpy of form.) <sup>[1]</sup> , -132 cal/mol ( $\Delta_f H^\circ$ ) <sup>[10]</sup>		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
-Δ <sub>ex</sub> U <sup>o</sup> [kJ kg <sup>-1</sup> ]	4,860		
T <sub>ex</sub> [K]	3,170		
p <sub>C-J</sub> [kbar]	186		

VoD [ $\text{m s}^{-1}$ ]	7,235 (@ 1.389 $\text{g cm}^{-3}$ )	7,580 (@ 1.50 $\text{g cm}^{-3}$ , calcd. BKW code) <sup>[8]</sup>	
$V_0$ [ $\text{L kg}^{-1}$ ]	913		

Melting enthalpy [J/g]	102.3 <sup>[11]</sup>
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DNDA-5 <sup>[6]</sup>	
Chemical formula	$\text{C}_3\text{H}_8\text{N}_4\text{O}_4$
Molecular weight [ $\text{g mol}^{-1}$ ]	164.13
Crystal system	Orthorhombic
Space group	Fdd2 (no. 43)
$a$ [ $\text{\AA}$ ]	20.815(5)
$b$ [ $\text{\AA}$ ]	43.427(5)
$c$ [ $\text{\AA}$ ]	6.236(5)
$\alpha$ [ $^\circ$ ]	90
$\beta$ [ $^\circ$ ]	90
$\gamma$ [ $^\circ$ ]	90
$V$ [ $\text{\AA}^3$ ]	5,637(5)
$Z$	32
$\rho_{\text{calc}}$ [ $\text{g cm}^{-3}$ ]	1.547
$T$ [K]	183

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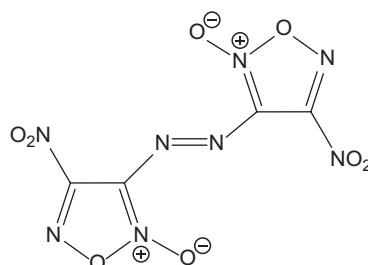
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**4,4'-Dinitro -3,3'-diazepnofuroxan**

Name [German, acronym]: Dinitrodiazepnofuroxan [DNAF]

Main (potential) use: high explosive

Structural formula:



	DNAF		
Formula	C <sub>4</sub> N <sub>8</sub> O <sub>8</sub>		
Molecular mass [g mol <sup>-1</sup> ]	288.09		
Appearance at RT	Transparent crystals (with peculiar luster under a microscope) <sup>[1]</sup> , red-orange needle crystals (from acetone/CHCl <sub>3</sub> ) <sup>[1]</sup>		
N [%]	38.90		
Ω(CO <sub>2</sub> ) [%]	0		
T <sub>m.p.</sub> [°C]	127–128 (dec. without melting, heating in capillary) <sup>[1]</sup> , 128 <sup>[3]</sup>		
T <sub>dec.</sub> [°C]	127–128 (heating in capillary, vigorous dec.) <sup>[1]</sup>		
ρ [g cm <sup>-3</sup> ]	2.002 (single crystal) <sup>[1]</sup> , 1.85 (powder pressed using dry-pressing technique, no heating, @ 3,800 kg/cm <sup>3</sup> ) <sup>[1]</sup> , 1.94 (hot-pressing @ 68 °C, with acetone/CHCl <sub>3</sub> solvent, 4,500 kg/cm <sup>2</sup> pressure for 10 min) <sup>[1]</sup> , overpressing @ pressures > 500 kg/cm <sup>2</sup> <sup>[1]</sup> , 2.02 (calcd.) <sup>[3]</sup>		
Heat of formation	186.6 kcal/mol ( $\Delta_f H^\circ$ , calcd.) <sup>[2]</sup> , 159.6 kcal/mol ( $\Delta_f H^\circ$ , calcd.) <sup>[2,3]</sup>		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
−Δ <sub>ex</sub> U <sup>0</sup> [kJ kg <sup>-1</sup> ]			1,788 <sup>[1]</sup>
T <sub>ex</sub> [K]			
p <sub>c-j</sub> [kbar]		467 (calcd.) <sup>[1]</sup>	

VoD [ $\text{m s}^{-1}$ ]		10,000 (@ 2.02 g $\text{cm}^{-3}$ (single crystal $\rho$ )) <sup>[1]</sup>  10,230 (@ 1.99 g $\text{cm}^{-3}$ , calcd.) <sup>[2]</sup>  10,000 (@ 2.00 g $\text{cm}^{-3}$ , calcd.) <sup>[2]</sup>  9,900 (@ 2.002 g $\text{cm}^{-3}$ , calcd) <sup>[2]</sup>  10,230 (@ 2.02 g $\text{cm}^{-3}$ , calcd.) <sup>[3]</sup>	9,700 (@ 1.94 g $\text{cm}^{-3}$ , ionization method using frequency meter, gage length no less than 10 mm) <sup>[1,2]</sup>  9,450 (@ 1.88 g $\text{cm}^{-3}$ , ionization method using frequency meter, gage length no less than 10 mm) <sup>[1,2]</sup>  9,000 (@ 1.77 g $\text{cm}^{-3}$ , ionization method using frequency meter, gage length no less than 10 mm) <sup>[1,2]</sup>
$V_0$ [ $\text{L kg}^{-1}$ ]			
Solubility [g/mL]	Recryst. from nitromethane <sup>[1]</sup>		

DNAF <sup>[1]</sup>	
Chemical formula	$\text{C}_4\text{N}_8\text{O}_8$
Molecular weight [g mol <sup>-1</sup> ]	288
Crystal system	Monoclinic
Space group	$P2_1/c$
$a$ [\mathring{A}]	6.240(1)
$b$ [\mathring{A}]	9.288(1)
$c$ [\mathring{A}]	24.752(4)
$\alpha$ [°]	90
$\beta$ [°]	91.11(1)
$\gamma$ [°]	90
$V$ [\mathring{A} <sup>3</sup> ]	1,433.6(4)
$Z$	6
$\rho_{\text{calc}}$ [g $\text{cm}^{-3}$ ]	2.002
$T$ [K]	

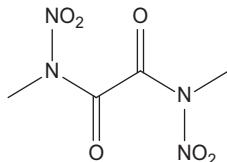
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## Dinitrodimethyloxamide

Name [German, acronym]: *N,N'-Dimethyl-N,N'-dinitrooxamide,*  
*N,N'-dinitro-N,N'-dimethyl oxamide*  
[initrodimethyloxamid, DNDMOA, DNDMO, MNO]

Main (potential) use: explosive

Structural formula:



	<b>Dinitrodimethyloxamide</b>		
Formula	C <sub>4</sub> H <sub>6</sub> N <sub>4</sub> O <sub>6</sub>		
Molecular mass [g mol <sup>-1</sup> ]	206.11		
Appearance at RT			
IS [J]	6 Nm <sup>[1]</sup> , H <sub>50</sub> = 79 cm <sup>[6]</sup> , Fl = 89% of TNT <sup>[7]</sup> , >100 cm (5 kg mass, Bruceton no. 3 apparatus) <sup>[2]</sup> , H <sub>50</sub> = 79 cm (2.5 kg mass, type 12 tool) <sup>[10]</sup> , H <sub>50</sub> ≥ 90 cm (design no. 3 apparatus) <sup>[13]</sup> , H <sub>50</sub> = 39 cm (design no. 5 apparatus) <sup>[13]</sup> , H <sub>50</sub> = 66.5 cm (design no. 12 apparatus, 89 units cf. TNT = 100 units) <sup>[13]</sup>		
N [%]	27.18		
Ω(CO <sub>2</sub> ) [%]	-38.8		
T <sub>m.p.</sub> [°C]	122–124 (dec.) <sup>[2]</sup> , 123 <sup>[7]</sup> , 124 (needles, recryst. from EtOH) <sup>[9]</sup> , 122.5–125 <sup>[11]</sup>		
ρ [g cm <sup>-3</sup> ]	1.523 <sup>[1]</sup> , 1.599 ± 0.06 (@ 293.15 K) <sup>[3]</sup> , 1.52 <sup>[7]</sup>		
Heat of formation	-302.6 kJ/mol (enthalpy of form., calcd., S-D method) <sup>[4]</sup> , -305.3 kJ/mol (enthalpy of form., exptl.) <sup>[4]</sup> , -322.2 kJ/mol (enthalpy of form., calcd., emp.) <sup>[4]</sup> , -74.5 kcal/mol (Δ <sub>f</sub> H <sup>o</sup> ) <sup>[2]</sup> , -1,482.0 kJ/kg (enthalpy of form.) <sup>[1]</sup>		
Heat of combustion	508.4 cal/mol <sup>[2,7]</sup> , 511.9 cal/mol (Q <sub>c</sub> ) <sup>[7]</sup>		
	Calcd. (EXPLO5)	Lit. values	Exptl.
-Δ <sub>ex</sub> U <sup>o</sup> [kJ kg <sup>-1</sup> ]	4,179	736 kcal/kg (calcd. heat of explosion @ 25 °C) <sup>[13]</sup>	
T <sub>ex</sub> [K]	3,129		

$p_{C_J}$ [kbar]	184		
VoD [ $\text{m s}^{-1}$ ]	7,025 (@ TMD)		5,050 (@ 1.0 $\text{g cm}^{-3}$ ) <sup>[7]</sup> 7,050 (@ 1.5 $\text{g cm}^{-3}$ ) <sup>[2,7,8]</sup> 6,760 (@ sp. gr. = 1.42 $\text{g cm}^{-3}$ ) <sup>[2]</sup> 7,100 (@ 1.48 $\text{g cm}^{-3}$ , confined) <sup>[1]</sup> 7,100 (@ 1.52 $\text{g cm}^{-3}$ ) <sup>[5]</sup> 23,600 ft/s (@ 1.5 g/mL) <sup>[11]</sup>
$V_0$ [ $\text{L kg}^{-1}$ ]	798		

Trauzl test [ $\text{cm}^3$ , % TNT]	115% TNT <sup>[2]</sup> , 110% PA <sup>[2]</sup> , 105% TNT <sup>[2,8]</sup> , 360 <sup>[12]</sup>
Sand test [g]	71% TNT <sup>[8]</sup>
Ballistic mortar test	116% TNT <sup>[2,7]</sup> , 129–135% TNT <sup>[8]</sup>
5 s explosion $T$ [ $^\circ\text{C}$ ]	No explosion @ 360 <sup>[11]</sup>
100 $^\circ\text{C}$ heat test [% mass loss]	Storage for 30 days @ 100 $^\circ\text{C}$ produces no red fumes <sup>[7,9]</sup>
International heat test	0.5% mass loss @ 75 $^\circ\text{C}$ <sup>[2]</sup>
Vacuum stability test [ $\text{cm}^3/\text{h}$ ]	5 cc gas evolved from 5 g sample in 5 h @ 120 $^\circ\text{C}$ <sup>[2]</sup>
Solubility [g/mL]	Very slightly soluble in $\text{H}_2\text{O}$ <sup>[9]</sup> , sparingly soluble in $\text{Et}_2\text{O}$ , $\text{CHCl}_3$ <sup>[9]</sup> , soluble in $\text{EtOH}$ <sup>[9]</sup>

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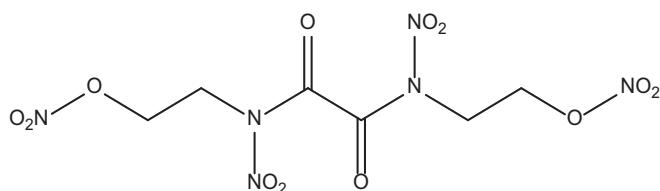
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## Dinitrodioxyethyloxamide dinitrate

Name [German, acronym]: Dinitrodioxyethyloxamide dinitrate, *N,N'*-dinitro-*N,N'*-dihydroxyethyloxamide dinitrate, *N,N'*-dinitro-*N,N'*-di(2-nitroethyl)-oxamide, *N,N'*-dinitro-*N,N'*-oxamide [dinitrodioxyethyloxamiddinitrat, dinitrodiethanoloxamiddinitrat, NENO]

Main (potential) use: Filler for explosives, tetryl substitute in boosters/detonators, component of bursting charges, high explosive

Structural formula:



	<b>NENO</b>															
Formula	C <sub>6</sub> H <sub>8</sub> N <sub>6</sub> O <sub>12</sub>															
Molecular mass [g mol <sup>-1</sup> ]	356.16															
Appearance at RT																
IS [J]	<p>Less than PETN, approx. that of RDX and tetryl and much less sensitive than PA or TNT<sup>[6]</sup>, 45 cm (ERL #3, sample in brass cup 0.308 in inside diameter, 0.01 in thick, 7/8 in height, 5 kg mass)<sup>[11]</sup>, 29 cm (ERL #12, sample on square of Flint paper, 2<sup>1</sup>/<sub>2</sub> kg mass)<sup>[11]</sup></p> <p>Design no. 3 apparatus<sup>[13]</sup>:</p> <table border="1"> <thead> <tr> <th>Drop height (cm)</th> <th>Trials</th> <th>% explosions</th> </tr> </thead> <tbody> <tr> <td>30</td> <td>20</td> <td>30</td> </tr> <tr> <td>40</td> <td>20</td> <td>35</td> </tr> <tr> <td>70</td> <td>20</td> <td>65</td> </tr> <tr> <td>80</td> <td>20</td> <td>85</td> </tr> </tbody> </table> <p>H<sub>50</sub> = 51 cm (design no. 3 apparatus, 5 kg hammer)<sup>[13]</sup>, H<sub>50</sub> = 42 cm (design no. 3 apparatus)<sup>[13]</sup>, H<sub>50</sub> = 16 cm (design no. 11 apparatus, 2.5 kg hammer)<sup>[13]</sup>, H<sub>50</sub> = 23 cm (design no. 12 apparatus, 31 units cf. TNT = 100 units)<sup>[13]</sup></p>	Drop height (cm)	Trials	% explosions	30	20	30	40	20	35	70	20	65	80	20	85
Drop height (cm)	Trials	% explosions														
30	20	30														
40	20	35														
70	20	65														
80	20	85														
N [%]	23.60															

$\Omega(\text{CO}_2)$ [%]	-18.0											
$T_{\text{m.p.}}$ [°C]	91–92 <sup>[1]</sup> , 88 <sup>[5]</sup> , 90–92 <sup>[6]</sup> , values reported in range 88.5–92 <sup>[9]</sup> , 95 (crystals from acetone) <sup>[10]</sup>											
$T_{\text{dec.}}$ [°C]	105 <sup>[6]</sup>											
$\rho$ [g cm <sup>-3</sup> ]	$1.779 \pm 0.06$ (@ 293.15 K) <sup>[2]</sup> , 1.72 <sup>[5]</sup> , 0.85–0.95 (bulk density) <sup>[6]</sup> , 1.60–1.64 (cast density) <sup>[6]</sup> , 1.706 (@ 22 °C, $\alpha$ -form) <sup>[6]</sup> , 1.686 (@ 22 °C, $\beta$ -form) <sup>[6]</sup> , 1.562 (@ 92.6 °C, $\beta$ -form) <sup>[6]</sup>											
Heat of formation	-581.6 kJ/mol (enthalpy of form., calcd., S-D method) <sup>[3]</sup> , -561.7 kJ/mol (enthalpy of form., exptl.) <sup>[3]</sup> , -494.7 kJ/mol (enthalpy of form., calcd., emp.) <sup>[3]</sup> , -1577.7 kJ/kg (enthalpy of form.) <sup>[5]</sup> , 132.20 kcal/mol ( $-\Delta H_f$ (heat of form. @ standard conditions) <sup>[12]</sup> )											
Heat of combustion	712 kcal/mol ( $Q_c^{\text{P}}$ ) <sup>[6]</sup> , 2024 cal/g (@ C') <sup>[6]</sup>  Exptl. heat of combustion data <sup>[12]</sup> :  <table border="1" style="margin-left: auto; margin-right: auto;"> <thead> <tr> <th><math>-\Delta U_{\text{B/M}}</math> (cal/g)</th> <th><math>-\Delta U_B</math> (kcal/mol)</th> <th><math>-\Delta U_R</math> (kcal/mol @ 1 atm and constant vol.)</th> <th><math>-\Delta H_R</math> (kcal/mol @ 1 atm and constant pressure)</th> </tr> </thead> <tbody> <tr> <td>2,003.91 ± 2.52</td> <td>713.74</td> <td>712.06</td> <td>707.91</td> </tr> </tbody> </table>				$-\Delta U_{\text{B/M}}$ (cal/g)	$-\Delta U_B$ (kcal/mol)	$-\Delta U_R$ (kcal/mol @ 1 atm and constant vol.)	$-\Delta H_R$ (kcal/mol @ 1 atm and constant pressure)	2,003.91 ± 2.52	713.74	712.06	707.91
$-\Delta U_{\text{B/M}}$ (cal/g)	$-\Delta U_B$ (kcal/mol)	$-\Delta U_R$ (kcal/mol @ 1 atm and constant vol.)	$-\Delta H_R$ (kcal/mol @ 1 atm and constant pressure)									
2,003.91 ± 2.52	713.74	712.06	707.91									
	Calcd. (EXPLO5)	Lit. values	Exptl.									
$-\Delta_{\text{ex}}U^\circ$ [kJ kg <sup>-1</sup> ]	4,965	1,211 kcal/kg (calcd. heat of explosion @ 25 °C) <sup>[13]</sup>	432 kcal/mol (@ 25 °C) <sup>[6]</sup> 1,211 kcal/kg <sup>[4]</sup>									
$T_{\text{ex}}$ [K]	3,482											
$p_{\text{CJ}}$ [kbar]	293											
$\text{VoD}$ [m s <sup>-1</sup> ]	8,222 (@ TMD)		7,800 (@ 1.63 g cm <sup>-3</sup> ) <sup>[7,11]</sup> 7,800–7,860 (@ 1.60–1.65 g cm <sup>-3</sup> , unconfined charge) <sup>[6]</sup> 5,400 (@ 1.0 g cm <sup>-3</sup> ) 25,100 ft/s (@ 1.5 g/mL) <sup>[9]</sup>									
$V_0$ [L kg <sup>-1</sup> ]	724											

Trauzl test [cm <sup>3</sup> , % TNT]	143% TNT <sup>[6]</sup> , 145% TNT <sup>[7]</sup>																				
Ballistic mortar test	131–135% TNT (@ 1.65 g cm <sup>-3</sup> , NENO) <sup>[6]</sup> , 129–135% TNT <sup>[7]</sup> , 135% TNT <sup>[11]</sup>																				
5 s explosion T [°C]	260–270 (25 mg sample) <sup>[6]</sup> , 260–270 (deflagrates) <sup>[9]</sup>  $T$ (°C) and explosion time (s), 25 mg sample <sup>[8]</sup> : <table border="1"> <thead> <tr> <th><math>T</math> (°C)</th> <th>Time (s)</th> <th><math>T</math> (°C)</th> <th>Time (s)</th> </tr> </thead> <tbody> <tr> <td>356</td> <td>0.080</td> <td>243</td> <td>1.69</td> </tr> <tr> <td>322</td> <td>0.183</td> <td>229</td> <td>2.70</td> </tr> <tr> <td>300</td> <td>0.316</td> <td>213</td> <td>4.75</td> </tr> <tr> <td>270</td> <td>0.650</td> <td>208</td> <td>No explosion</td> </tr> </tbody> </table>	$T$ (°C)	Time (s)	$T$ (°C)	Time (s)	356	0.080	243	1.69	322	0.183	229	2.70	300	0.316	213	4.75	270	0.650	208	No explosion
$T$ (°C)	Time (s)	$T$ (°C)	Time (s)																		
356	0.080	243	1.69																		
322	0.183	229	2.70																		
300	0.316	213	4.75																		
270	0.650	208	No explosion																		
Abel heat test	45–50 s @ 80 °C (material before recryst.) <sup>[10]</sup> , 6 min 13 s @ 80 °C (recryst. material) <sup>[10]</sup>																				
Vacuum stability test [cm <sup>3</sup> /h]	4 cc gas evolved in 6 h @ 100 °C <sup>[6]</sup>																				
Thermal stability	Stable under slightly elevated $T$ and considerable humidity <sup>[9]</sup>																				
Solubility [g/mL]	Soluble in acetone and ethyl acetate <sup>[10]</sup> , slightly soluble in benzene <sup>[10]</sup> , practically insoluble in CCl <sub>4</sub> , CHCl <sub>3</sub> and EtOH <sup>[10]</sup>																				

Two polymorphs of NENO known<sup>[6]</sup>:

- (i) α-form, needles, stable @ RT, slow recryst. from chloroform <38 °C<sup>[6]</sup>
- (ii) β-form, monoclinic, recryst. from chloroform >38 °C<sup>[6]</sup>

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- [9] *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**.

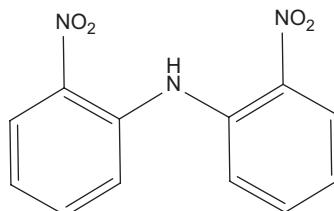
- [10] *Handbook of Foreign Explosives*, U. S. Materiel Command, US Army Foreign Science and Technology Center, Washington, D. C., USA, October **1965**.
- [11] *Summary Technical Report of Division 8, NDRC, Volume 1, The Preparation and Testing of Explosives*, Office of Scientific Research and Development, National Defense Research Committee, Washington D. C., USA, **1946**.
- [12] 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**.
- [13] H. D. Mallory, *The Development of Impact Sensitivity Tests at the Explosives Research Laboratory Bruceton, Pennsylvania During the Years 1941–1945*, NAVORD Report 4236, US Naval Ordnance Laboratory, White Oak, Maryland, USA, 16th March **1956**.

## 2,2'-Dinitrodiphenylamine

Name [German, acronym]: 2,2'-Dinitrodiphenylamine [2,2'-dinitrodiphenylamin]

Main (potential) use: stabilizer

Structural formula:



	2,2'-Dinitrodiphenylamine	
Formula	C <sub>12</sub> H <sub>9</sub> N <sub>3</sub> O <sub>4</sub>	
Molecular mass [g mol <sup>-1</sup> ]	259.22	
N [%]	16.21	
Ω(CO <sub>2</sub> ) [%]	-151.2	
T <sub>m.p.</sub> [°C]	172.3 ± 0.5 <sup>[1]</sup>	
ρ [g cm <sup>-3</sup> ]	1.446 ± 0.06 (@ 293.15 K) <sup>[2]</sup>	
Heat of formation	29.2 kJ/mol (enthalpy of form., calcd., emp.) <sup>[3]</sup> , 22.9 kJ/mol (enthalpy of form., exptl.) <sup>[3]</sup> , 38 kJ/mol (enthalpy of form., calcd., S-D method) <sup>[3]</sup>	
	Calcd. (K-J)	Exptl.
-Δ <sub>ex</sub> U <sup>o</sup> [kJ kg <sup>-1</sup> ]		
T <sub>ex</sub> [K]		
p <sub>C-J</sub> [GPa]		
VoD [m s <sup>-1</sup> ]		
V <sub>0</sub> [L kg <sup>-1</sup> ]		

[1] D. Trache, K. Khimeche, A. Dahmani, *International Journal of Thermophysics*, **2013**, *34*, 226–239.

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

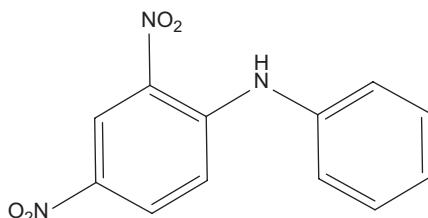
[3] B. Nazari, M. H. Keshavarz, M. Hamadanian, S. Mosavi, A. R. Ghaedsharafi, H. R. Pouretedal, *Fluid Phase Equilibria*, **2016**, *408*, 248–258.

## **2,4-Dinitrodiphenylamine**

Name [German, acronym]: 2,4-Dinitrodiphenylamine [2,4-dinitrodiphenylamin]

Main (potential) use: stabilizer

**Structural formula:**



2,4-Dinitrodiphenylamine	
Formula	C <sub>12</sub> H <sub>9</sub> N <sub>3</sub> O <sub>4</sub>
Molecular mass [g mol <sup>-1</sup> ]	259.22
N [%]	16.21
Ω(CO <sub>2</sub> ) [%]	-151.2
T <sub>m.p.</sub> [°C]	159 <sup>[1]</sup> , 156 (DSC @ 10 °C/min) <sup>[4]</sup>
T <sub>dec.</sub> [°C]	200 (onset), 325 (peak) (DSC @ 10 °C/min) <sup>[4]</sup>
ρ [g cm <sup>-3</sup> ]	1.446 ± 0.06 (@ 293.15 K) <sup>[2]</sup>
Heat of formation	29.2 kJ/mol (enthalpy of form., calcd., emp.) <sup>[3]</sup> , 22.5 kJ/mol (enthalpy of form., exptl.) <sup>[3]</sup> , 38 kJ/mol (enthalpy of form., calcd., S-D method) <sup>[3]</sup>
Calcd. (K-J)	Exptl.
-Δ <sub>ex</sub> U° [kJ kg <sup>-1</sup> ]	
T <sub>ex</sub> [K]	
p <sub>C-J</sub> [kbar]	
VoD [m s <sup>-1</sup> ]	
V <sub>0</sub> [L kg <sup>-1</sup> ]	

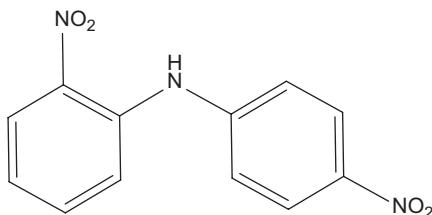
- [1] "PhysProp" data were obtained from Syracuse Research Corporation of Syracuse, New York (US).
- [2] Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994–2017 ACD/Labs).
- [3] B. Nazari, M. H. Keshavarz, M. Hamadanian, S. Mosavi, A. R. Ghaedsharafi, H. R. Pouretedal, *Fluid Phase Equilibria*, **2016**, *408*, 248–258.
- [4] J. Hernández-Paredes, R. C. Carillo-Torres, O. Hernández-Negrete, R. R. Sotelo-Mundo, D. Glossmann-Mitnik, H. E. Esparza-Ponce, *J. Molec. Struct.*, **2017**, *1141*, 53–63.

## 2,4'-Dinitrodiphenylamine

Name [German, acronym]: 2,4'-Dinitrodiphenylamine [2,4'-dinitrodiphenylamin]

Main (potential) use: stabilizer

Structural formula:



2,4'-Dinitrodiphenylamine	
Formula	C <sub>12</sub> H <sub>9</sub> N <sub>3</sub> O <sub>4</sub>
Molecular mass [g mol <sup>-1</sup> ]	259.22
N [%]	16.21
Ω(CO <sub>2</sub> ) [%]	-151.2
T <sub>m.p.</sub> [°C]	219–220 <sup>[1]</sup>
ρ [g cm <sup>-3</sup> ]	1.446 ± 0.06 (@ 293.15 K) <sup>[2]</sup>
Heat of formation	88.3 kJ/kg (enthalpy of form.) <sup>[3]</sup>
Calcd. (K-J)	Exptl.
-Δ <sub>ex</sub> U° [kJ kg <sup>-1</sup> ]	
T <sub>ex</sub> [K]	
p <sub>C-J</sub> [kbar]	
VoD [m s <sup>-1</sup> ]	
V <sub>0</sub> [L kg <sup>-1</sup> ]	

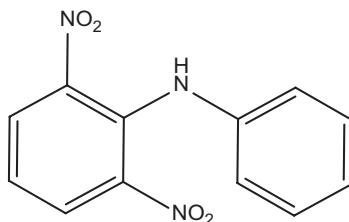
- [1] A. R. Katritzky, S. G. P. Plant, *J. Chem. Soc.*, **1953**, 412–416.  
[2] Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994–2017 ACD/Labs).  
[3] R. Meyer, J. Köhler, A. Homburg, *Explosives*, 7th edn., Wiley-VCH, Weinheim, **2016**, p. 105.

## 2,6-Dinitrodiphenylamine

Name [German, acronym]: 2,6-Dinitrodiphenylamine [2,6-dinitrodiphenylamin]

Main (potential) use: stabilizer

Structural formula:



	2,6-Dinitrodiphenylamine	
Formula	$\text{C}_{12}\text{H}_9\text{N}_3\text{O}_4$	
Molecular mass [g mol <sup>-1</sup> ]	259.22	
N [%]	16.21	
$\Omega(\text{CO}_2)$ [%]	-151.2	
$T_{\text{m.p.}}$ [°C]	107–108 <sup>[1]</sup>	
$\rho$ [g cm <sup>-3</sup> ]	$1.446 \pm 0.06$ (@ 293.15 K) <sup>[2]</sup>	
Heat of formation	88.3 kJ/kg (enthalpy of form.) <sup>[3]</sup>	
	Calcd. (K-J)	Exptl.
$-\Delta_{\text{ex}}U^\circ$ [kJ kg <sup>-1</sup> ]		
$T_{\text{ex}}$ [K]		
$p_{\text{C-J}}$ [kbar]		
VoD [m s <sup>-1</sup> ]		
$V_0$ [L kg <sup>-1</sup> ]		

[1] W. Borsche, D. Rantscheff, *Justus Liebigs Annalen der Chemie*, **1911**, 379, 152–182.

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

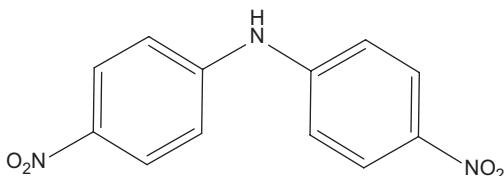
[3] R. Meyer, J. Köhler, A. Homburg, *Explosives*, 7th edn., Wiley-VCH, Weinheim, **2016**, p. 105.

## 4,4'-Dinitrodiphenylamine

Name [German, acronym]: 4,4'-Dinitrodiphenylamine [4,4'-dinitrodiphenylamin]

Main (potential) use: stabilizer

Structural formula:



	4,4'-Dinitrodiphenylamine
Formula	$\text{C}_{12}\text{H}_9\text{N}_3\text{O}_4$
Molecular mass [g mol <sup>-1</sup> ]	259.22
N [%]	16.21
$\Omega(\text{CO}_2)$ [%]	-151.2
$T_{\text{m.p.}}$ [°C]	216–218 <sup>[1]</sup>
$\rho$ [g cm <sup>-3</sup> ]	$1.446 \pm 0.06$ (@ 293.15 K) <sup>[2]</sup>
Heat of formation	88.3 kJ/kg (enthalpy of form.) <sup>[3]</sup>
	Calcd. (K-J)
	Exptl.
$-\Delta_{\text{ex}}U^\circ$ [kJ kg <sup>-1</sup> ]	
$T_{\text{ex}}$ [K]	
$p_{\text{C-J}}$ [kbar]	
VoD [m s <sup>-1</sup> ]	
$V_0$ [L kg <sup>-1</sup> ]	

[1] K. Haga, K. Iwaya, R. Kaneko, *Bull. Chem. Soc. Japan*, **1986**, 59, 803–807.

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

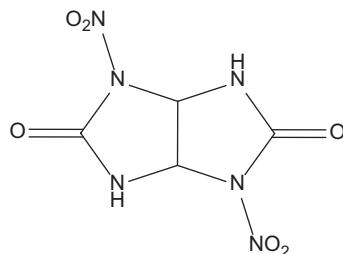
[3] R. Meyer, J. Köhler, A. Homburg, *Explosives*, 7th edn., Wiley-VCH, Weinheim, **2016**, p. 105.

## 1,4-Dinitroglycolurile

Name [German, acronym]: 1,4-Dinitroglycolurile, 1,4-dinitro-tetrahydro-imidazo(4,5-d)imidazole-2,5(1H,3H)-dione, 2,6-dinitro-2,4,6,8-tetraazabicyclo[3.3.0]octane-3,7-dione [DINGU, DNGU]

Main (potential) use: Of interest as self-remediating explosive<sup>[2]</sup>

Structural formula:



	<b>DINGU</b>																														
Formula	C <sub>4</sub> H <sub>4</sub> N <sub>6</sub> O <sub>6</sub>																														
Molecular mass [g mol <sup>-1</sup> ]	232.11																														
Appearance at RT	Rod-shaped crystals of 10–100 µm length (crude product) <sup>[20]</sup> , diamond-shaped crystals on recryst. from adding hot nitric acid soln. to cold water <sup>[20]</sup>																														
IS [J]	<p>5.55<sup>[1]</sup>, 5.55 (first reaction)<sup>[6,14]</sup>, 24.61 (sound)<sup>[6,14]</sup>, 0.8 ((no units) based on TNT = 1)<sup>[8]</sup>, H<sub>50</sub> = 100 cm<sup>[9]</sup>, 5–6 Nm<sup>[2]</sup>, 0.5–0.6 kgm<sup>[11]</sup></p> <p>Type 12 test = 40 mg sample placed in conical pile on garnet paper, 2.5 kg mass; type 12B test = sample placed on bare anvil, 2.5 kg mass, data from ref, Bruceton method, H<sub>50</sub> values<sup>[20]</sup>:</p> <table border="1"> <thead> <tr> <th>Particle size (µm)</th> <th>5</th> <th>1–30</th> <th>20–40</th> <th>30–60</th> <th>30–100</th> </tr> </thead> <tbody> <tr> <td>Crystal habit</td> <td></td> <td></td> <td></td> <td>Diamond</td> <td>Rod</td> </tr> <tr> <td>Impact sensitivity</td> <td></td> <td></td> <td></td> <td></td> <td></td> </tr> <tr> <td>Type 12 (cm)</td> <td>88</td> <td>101</td> <td>108</td> <td>108</td> <td>125</td> </tr> <tr> <td>Type 12B (cm)</td> <td>78</td> <td>153</td> <td>175</td> <td>204</td> <td>212</td> </tr> </tbody> </table>	Particle size (µm)	5	1–30	20–40	30–60	30–100	Crystal habit				Diamond	Rod	Impact sensitivity						Type 12 (cm)	88	101	108	108	125	Type 12B (cm)	78	153	175	204	212
Particle size (µm)	5	1–30	20–40	30–60	30–100																										
Crystal habit				Diamond	Rod																										
Impact sensitivity																															
Type 12 (cm)	88	101	108	108	125																										
Type 12B (cm)	78	153	175	204	212																										
FS [N]	20–300 <sup>[2]</sup> , p <sub>fr,LL</sub> = 300 MPa <sup>[10]</sup> , p <sub>fr,50%</sub> = 450 MPa <sup>[10]</sup> , 20–30 kg pistil load <sup>[11]</sup>																														



		<p>8,670 (@ 1.98 g cm<sup>-3</sup>, ΔH<sub>f</sub> = -433 kJ/mol, calcd., JAGUAR)<sup>[16]</sup></p> <p>Calcd., Fortran BKW equation of state<sup>[20]</sup>:</p> <table border="1"> <thead> <tr> <th><math>\rho</math> (g/cm<sup>3</sup>)</th><th>1.75</th><th>1.85</th><th>1.94</th><th>1.98</th></tr> </thead> <tbody> <tr> <td>CJ pressure (GPa)</td><td>26.5</td><td>30.6</td><td>34.7</td><td>36.7</td></tr> <tr> <td>VoD (m/s)</td><td>7,890</td><td>8,300</td><td>8,680</td><td>8,870</td></tr> </tbody> </table>	$\rho$ (g/cm <sup>3</sup> )	1.75	1.85	1.94	1.98	CJ pressure (GPa)	26.5	30.6	34.7	36.7	VoD (m/s)	7,890	8,300	8,680	8,870	<p>7,580 (@ 1.75 g cm<sup>-3</sup>, confined)<sup>[2]</sup></p> <p>DINGU is a class 2 explosive in that the VoD stops increasing linearly with density at high densities<sup>[20]</sup></p>
$\rho$ (g/cm <sup>3</sup> )	1.75	1.85	1.94	1.98														
CJ pressure (GPa)	26.5	30.6	34.7	36.7														
VoD (m/s)	7,890	8,300	8,680	8,870														
$V_0$ [L kg <sup>-1</sup> ]	696																	

Critical temperature [°C]	204 (modified Henkin-critical-temperature method, 40 mg sample pressed into cartridge and confined lightly by metal cup, Wood's metal bath, timed to explosion) <sup>[20]</sup> , 210 (modified Henkin-critical-temperature method, 40 mg sample pressed into cartridge and confined lightly by metal cup, Wood's metal bath, timed to explosion, deuterated DINGU) <sup>[20]</sup>								
SSGT [cm]	SSGT of DINGU (donor = PBX 9407, acceptor explosive = 12.7 mm diameter, 38 mm length, assembly held together by Lucite) <sup>[20]</sup> :								
	<table border="1"> <thead> <tr> <th></th> <th><math>\rho</math> (g/cm<sup>3</sup>)</th> <th>Voids (%)</th> <th>G<sub>50</sub> (mm)</th> </tr> </thead> <tbody> <tr> <td>DINGU</td> <td>1.76</td> <td>11</td> <td>0.18</td> </tr> </tbody> </table>		$\rho$ (g/cm <sup>3</sup> )	Voids (%)	G <sub>50</sub> (mm)	DINGU	1.76	11	0.18
	$\rho$ (g/cm <sup>3</sup> )	Voids (%)	G <sub>50</sub> (mm)						
DINGU	1.76	11	0.18						
5 s explosion T [°C] Explosion T [°C]	180 (ARC sample bomb, 0.5 g sample, analyzed in 5 °C steps from 50 to 350 °C until it begins to self-heat and violent gas explosion >180 °C) <sup>[20]</sup>								
Vacuum stability test [cm <sup>3</sup> /h]	STANAG 4147 test 1B, total gas evolved after 40 h (@ 100 °C, values in cc): 0.4744 <sup>[18]</sup> , 0.5 mL/g gas (0.2 g sample @ 120 °C for 48 h) <sup>[20]</sup>								
Thermal stability	Pipe blown into 10 cm fragments @ 190 °C in larger, confined pipe test <sup>[20]</sup>								
Vapor pressure [atm @ °C]	$2.54 \times 10^{-13}$ Torr (est.) @ 25 °C <sup>[17]</sup> , $2.06 \times 10^{-10}$ Torr (est.) @ 70 °C <sup>[17]</sup> , $5.40 \times 10^{-8}$ Torr (est.) @ 100 °C <sup>[17]</sup>								
Burn rate [mm/s]	<p>Burning rate test data (binder = Kraton oil)<sup>[20]</sup>:</p> <table border="1"> <thead> <tr> <th>DINGU</th> <th>Burn rate (mm/s)</th> </tr> </thead> <tbody> <tr> <td>Burn rate (mm/s) 50/50 binder 6.89 MPa (1,000 psi)</td> <td>5–6.6</td> </tr> <tr> <td>Approx. burn rate (mm/s) 95/5 HE/binder ambient pressure</td> <td>0.4</td> </tr> </tbody> </table>	DINGU	Burn rate (mm/s)	Burn rate (mm/s) 50/50 binder 6.89 MPa (1,000 psi)	5–6.6	Approx. burn rate (mm/s) 95/5 HE/binder ambient pressure	0.4		
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Burn rate (mm/s) 50/50 binder 6.89 MPa (1,000 psi)	5–6.6								
Approx. burn rate (mm/s) 95/5 HE/binder ambient pressure	0.4								

Solubility [g/mL]	$1.4 \times 10^{-1}$ mg/mL in H <sub>2</sub> O (hydrolysis) <sup>[17]</sup>																																																																	
Hygroscopicity	Hydrolysis <sup>[17]</sup>																																																																	
Compatibility	<p>Hydrolyzes in H<sub>2</sub>O, half-life = 90 min<sup>[17]</sup></p> <p>VTS compatibility (STANAG 4147 test 1B, 2.5 g of compound 1 mixed with 2.5 g of compound 2, total gas evolved after 40 h @ 100 °C, values in cc)<sup>[18]</sup>: 0.4569 (TNBA), – (DNMT), 1.5223 (PiPE), 2.0563 (DNP), 0.6147 (LLM-105), 0.4653 (HK-56), – (HMX) concluding that all are compatible with DNGU<sup>[18]</sup></p>																																																																	
$\Delta H_{dec}$ [J/g]	1,051 (DSC @ 10 °C/min, hermetic pan, pinhole lid) <sup>[17]</sup> , 896.0 (DSC @ 10 °C/min, standard pan) <sup>[17]</sup>																																																																	
$\Delta H_{vap}$ [kJ/mol]	151.2 (est.) <sup>[17]</sup>																																																																	
$K_{ow}$	0.253 <sup>[17]</sup> , $\log K_{ow} = -0.60$ <sup>[17]</sup>																																																																	
$K_{oc}$	1,482 (predicted) <sup>[17]</sup>																																																																	
Plate dent test	<p>Unconfined tests correlated to detonation pressure, samples pressed to 1.27, 2.54 or 3.16 cm diameter placed onto 5.1 cm thick, 15 cm × 15 cm square, cold-rolled steel plate; resulting dent is compared to those of standard explosives<sup>[20]</sup>:</p> <table border="1"> <thead> <tr> <th>Formulation</th> <th>Test diameter (mm)</th> <th><math>\rho</math> (g/cm<sup>3</sup>)</th> <th>% TMD</th> <th>Indicated pressure (GPa)</th> </tr> </thead> <tbody> <tr> <td rowspan="5">Estane 1</td> <td rowspan="5">25.4</td> <td>1.715</td> <td>90.3</td> <td>18.8</td> </tr> <tr> <td>1.795</td> <td>94.5</td> <td>21.6</td> </tr> <tr> <td>1.825</td> <td>96.0</td> <td>18.4</td> </tr> <tr> <td>1.849</td> <td>97.3</td> <td>10.4</td> </tr> <tr> <td>1.867</td> <td>98.3</td> <td>Failed</td> </tr> <tr> <td></td> <td></td> <td></td> <td></td> </tr> <tr> <td rowspan="2">Estane 1</td> <td rowspan="2">41.3</td> <td>1.828</td> <td>96.2</td> <td>25.2</td> </tr> <tr> <td>1.848</td> <td>97.3</td> <td>25.2</td> </tr> <tr> <td></td> <td></td> <td></td> <td></td> </tr> <tr> <td rowspan="6">Estane 2</td> <td rowspan="6">25.4</td> <td>1.722</td> <td>90.0</td> <td>20.9</td> </tr> <tr> <td>1.798</td> <td>94.0</td> <td>22.9</td> </tr> <tr> <td>1.817</td> <td>95.0</td> <td>23.6</td> </tr> <tr> <td>1.833</td> <td>96.0</td> <td>23.8</td> </tr> <tr> <td>1.855</td> <td>97.0</td> <td>24.2</td> </tr> <tr> <td>1.879</td> <td>98 +</td> <td>23.5</td> </tr> <tr> <td></td> <td></td> <td></td> <td></td> </tr> </tbody> </table>				Formulation	Test diameter (mm)	$\rho$ (g/cm <sup>3</sup> )	% TMD	Indicated pressure (GPa)	Estane 1	25.4	1.715	90.3	18.8	1.795	94.5	21.6	1.825	96.0	18.4	1.849	97.3	10.4	1.867	98.3	Failed					Estane 1	41.3	1.828	96.2	25.2	1.848	97.3	25.2					Estane 2	25.4	1.722	90.0	20.9	1.798	94.0	22.9	1.817	95.0	23.6	1.833	96.0	23.8	1.855	97.0	24.2	1.879	98 +	23.5				
Formulation	Test diameter (mm)	$\rho$ (g/cm <sup>3</sup> )	% TMD	Indicated pressure (GPa)																																																														
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Estane 2	41.3	1.722	90.0	20.9	
		1.798	94.0	24.0	
		1.836	96.0	24.6	
		1.875	98.0	24.8	
Exon 1	25.4	1.857	96.0	25.5	
		1.892	98.0	26.2	
Exon 1	41.3	1.856	96.0	27.0	
		1.877	97.0	27.6	

Estane 1 = 95/4/1 wt.% DINGU/Estane/KR138-S; Estane 2 = 96/3/1 wt.% DINGU/Estane/KR138-S; Exon 1 = 94/5/1 wt.% DINGU/Exon 461/KR138-S.

	DINGU <sup>[19]</sup>	DINGU <sup>[4]</sup>
Chemical formula	C <sub>4</sub> H <sub>4</sub> N <sub>6</sub> O <sub>6</sub>	C <sub>4</sub> H <sub>4</sub> N <sub>6</sub> O <sub>6</sub>
Molecular weight [g mol <sup>-1</sup> ]	232.1	232.1
Crystal system	Triclinic	Triclinic
Space group	P1	P-1 (no. 2)
<i>a</i> [Å]	10.738	6.392(5)
<i>b</i> [Å]	10.870	6.984(5)
<i>c</i> [Å]	15.027	9.228(6)
$\alpha$ [°]	106.04	103.38(6)
$\beta$ [°]	93.57	101.57(6)
$\gamma$ [°]	90.47	96.64(6)
<i>V</i> [Å <sup>3</sup> ]		386.912
<i>Z</i>		2
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]		1.992
<i>T</i> [K]		295
	Recryst. from DMSO	Crystal grown from conc. nitric acid

Rod-shaped crystals of 10–100 µm length (crude product)<sup>[20]</sup>, diamond-shaped crystals on recryst. from adding hot nitric acid soln. to cold water<sup>[20]</sup>, the diamond-shaped crystals are the same polymorph as the rod-shaped crystals.<sup>[20]</sup>

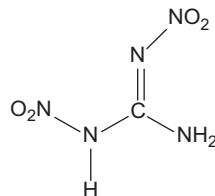
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## 1,2-Dinitroguanidine

Name [German, acronym]: Dinitroguanidine, [1,2-dinitroguanidin, DNQ]

Main (potential) use: explosive, gas generant

Structural formula:



	1,2-Dinitroguanidine		
Formula	$\text{CH}_3\text{N}_5\text{O}_4$		
Molecular mass [g mol <sup>-1</sup> ]	149.08		
Appearance at RT	Colorless crystalline solid <sup>[3]</sup>		
IS [J]	$H_{50\%} = 60 \text{ cm}$ (5 kg mass, 30 mg sample, K-44-II Russian drop-weight impact machine) <sup>[2]</sup> , $H_{100\%} = 22 \text{ cm}$ (5 kg mass, 30 mg sample, K-44-II Russian drop-weight impact machine) <sup>[2]</sup>		
N [%]	46.98		
$\Omega(\text{CO}_2)$ [%]	5.4		
$T_{\text{m.p.}}$ [°C]	168–169 <sup>[3]</sup>		
$T_{\text{dec.}}$ [°C]			
$\rho$ [g cm <sup>-3</sup> ]	1.884 (crystal @ 298 K) <sup>[1]</sup> , 1.906 <sup>[4]</sup>		
Heat of formation	0 kJ mol <sup>-1</sup> ( $\Delta_f H^\circ$ ) <sup>[2,4]</sup>		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{\text{ex}} U^\circ$ [kJ kg <sup>-1</sup> ]	5.11 MJ/kg ( $Q_{\text{expl.}}$ , @ 1.88 g cm <sup>-3</sup> , calcd., BKW) <sup>[2]</sup>  $Q_{\text{cal}} = 4979 \text{ kJ/kg}$ <sup>[4]</sup>		
$T_{\text{ex}}$ [K]	1820 (calcd., BKW-RDX, @ 1.88 g cm <sup>-3</sup> ) <sup>[2]</sup>  3,784 (calcd., BKW-C, @ 1.88 g cm <sup>-3</sup> ) <sup>[2]</sup>		

$p_{C_J}$ [kbar]		$365 \pm 4.4\%$ (@ 1.88 g cm <sup>-3</sup> , calcd. BKW) <sup>[2]</sup>	360 (@ 1.87 g cm <sup>-3</sup> ) <sup>[2]</sup>
VoD [m s <sup>-1</sup> ]		$9,100 \pm 3.0\%$ (@ 1.88 g cm <sup>-3</sup> , calcd. BKW) <sup>[2]</sup>  9,200 (@ 1.906 g cm <sup>-3</sup> ) <sup>[4]</sup>	9,200 (@ 1.87 g cm <sup>-3</sup> ) <sup>[2]</sup>
$V_0$ [L kg <sup>-1</sup> ]		$0.79 \pm 0.05\%$ m <sup>3</sup> /kg (@ 1.88 g cm <sup>-3</sup> , calcd. BKW) <sup>[2]</sup>	
Initiation by impact critical parameters			$620 < p_{cr.} < 730$ MPa <sup>[2]</sup> , $T_{cr.} = 568$ °C <sup>[2]</sup> , $0.42 > h_{cr.} > 0.35$ mm <sup>[2]</sup>
LSGT [cm]	$p_{cr.} = 1.2$ GPa (critical pressure of detonation initiation, calcd., LSGT) <sup>[4]</sup>		
Solubility [g/mL]	Soluble in EtOH and acetic acid <sup>[3]</sup> , moderately soluble in H <sub>2</sub> O and organic solvents <sup>[3]</sup> , saturated aqueous soln. = 53 g/L @ 20 °C <sup>[3]</sup> saturated ethyl acetate soln. = 86 g/L @ 20 °C <sup>[3]</sup> , good solubility in warm H <sub>2</sub> O and warm organic solvents such as EtOH, ethyl acetate, acetone, acetonitrile <sup>[3]</sup> , much less soluble in aromatic hydrocarbons and chloroalkanes <sup>[3]</sup>		
Compatibility	Dec. in sulfuric acid <sup>[3]</sup> , deprotonation by aqueous solns. of group 1 metal hydroxides <sup>[3]</sup>		
$\Delta H^\circ_{subl.}$ [kJ/mol]	123.6 ± 2.2 <sup>[2]</sup>		
$pK_a$	diacid: 1.11, ~ 11.5 <sup>[3]</sup>		

1,2-Dinitroguanidine <sup>[1,2]</sup>	
Chemical formula	CH <sub>3</sub> N <sub>5</sub> O <sub>4</sub>
Molecular weight [g mol <sup>-1</sup> ]	149.08
Crystal system	Orthorhombic
Space group	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub> (no. 19)
$a$ [\AA]	9.6465(6)
$b$ [\AA]	10.7694(7)
$c$ [\AA]	5.0583(3)
$\alpha$ [°]	90
$\beta$ [°]	90
$\gamma$ [°]	90

$V [\text{\AA}^3]$	525.49(6)
Z	4
$\rho_{\text{calc}} [\text{g cm}^{-3}]$	1.884
T [K]	293

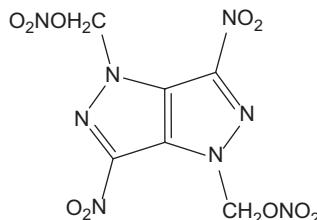
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## 1,4-Dinitromethyl-3,6-dinitropyrazolo[4,3-*c*]pyrazole

Name [German, acronym]: 1,4-Dinitromethyl-3,6-dinitropyrazolo[4,3-*c*]pyrazole  
 [1,4-dinitromethyl-3,6-dinitropyrazolo[4,3-*c*]pyrazol]

Main (potential) use: high explosive

Structural formula:



	1,4-Dinitromethyl-3,6-dinitropyrazolo[4,3- <i>c</i> ]pyrazole		
Formula	$C_6H_4N_8O_{10}$		
Molecular mass [g mol <sup>-1</sup> ]	348.17		
Appearance at RT	Yellowish solid <sup>[1]</sup>		
IS [J]	12 (BAM) <sup>[1]</sup>		
FS [N]	160 (BAM) <sup>[1]</sup>		
N [%]	32.19		
$\Omega(CO_2)$ [%]	-18.4		
$T_{dec.}$ [°C]	208 <sup>[1]</sup>		
$\rho$ [g cm <sup>-3</sup> ]	1.83 (X-ray @ 296 K) <sup>[1]</sup>		
Heat of formation	18.8 kJ/mol ( $\Delta H_f$ , calcd.) <sup>[1]</sup>		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{ex}U^\circ$ [kJ kg <sup>-1</sup> ]			
$T_{ex}$ [K]			
$p_{C-J}$ [kbar]		32.8 GPa (@ 1.83 g cm <sup>-3</sup> , calcd., K-J) <sup>[1]</sup>	
VoD [m s <sup>-1</sup> ]		8,480 (@ 1.83 g cm <sup>-3</sup> , calcd., K-J) <sup>[1]</sup>	
$V_0$ [L kg <sup>-1</sup> ]			

	<b>1,4-Dinitromethyl-3,6-dinitropyrazolo[4,3-c]pyrazole<sup>[1]</sup></b>
Chemical formula	C <sub>6</sub> H <sub>4</sub> N <sub>8</sub> O <sub>10</sub>
Molecular weight [g mol <sup>-1</sup> ]	348.17
Crystal system	Triclinic
Space group	<i>P</i> -1
<i>a</i> [Å]	7.743(4)
<i>b</i> [Å]	8.302(5)
<i>c</i> [Å]	10.605(6)
$\alpha$ [°]	85.500(11)
$\beta$ [°]	78.807(10)
$\gamma$ [°]	71.153(9)
<i>V</i> [Å <sup>3</sup> ]	632.8(6)
<i>Z</i>	2
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.827
<i>T</i> [K]	296

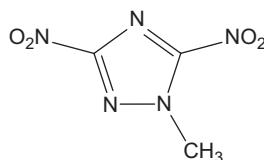
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## Dinitromethyltriazole

Name [German, acronym]: 1-Methyl-3,5-dinitro-1*H*-1,2,4-triazole,  
[dinitromethyltriazol, DNMT]

Main (potential) use: Investigated as possible new melt-pour energetic material<sup>[1]</sup>, used as melt-cast binder to replace TNT<sup>[4]</sup>

Structural formula:



	<b>DNMT</b>		
Formula	C <sub>3</sub> H <sub>3</sub> N <sub>5</sub> O <sub>4</sub>		
Molecular mass [g mol <sup>-1</sup> ]	173.09		
Appearance at RT	White crystals on recryst. from isopropanol <sup>[3]</sup>		
IS [J]	>100 cm (ERL apparatus) <sup>[1,4]</sup> , insensitive to impact <sup>[2]</sup> , detonates when 2 kg mass dropped from 70 cm onto 35 mg sample <sup>[3]</sup> , 92.7 cm (premelt, ERL apparatus) <sup>[4]</sup> , 171.0 cm (after melting and resolidifying, ERL apparatus) <sup>[4]</sup> Navy method: 92.7 cm (premelt) <sup>[1]</sup> , 171.0 cm (postmelt) <sup>[1]</sup>		
FS [N]	>252 (BAM) <sup>[1,4]</sup> , insensitive to friction <sup>[2]</sup>		
ESD [J]	>0.25 <sup>[1,4]</sup> , insensitive to ESD <sup>[2]</sup>		
N [%]	40.46		
Ω(CO <sub>2</sub> ) [%]	-32.4		
T <sub>m.p.</sub> [°C]	~95 <sup>[1]</sup> , 95.7 (endo peak max, DSC @ 5 °C/min) <sup>[1]</sup> , 95 <sup>[2]</sup> , 98–98.5 (crystals from isopropanol) <sup>[3]</sup> , 88.94 (endo onset), 95.53 (endo, peak max) (DSC @ 10 °C/min) <sup>[4]</sup>		
T <sub>phase transition</sub> [°C]	No polymorphs observed on heating <sup>[4]</sup> , DNMT suggested to be amorphous rather than crystalline after melting and resolidifying <sup>[4]</sup>		
T <sub>dec.</sub> [°C]	260.6 (exo, onset), 280.0 (exo, peak max) (DSC @ 5 °C/min) <sup>[1]</sup>		
ρ [g cm <sup>-3</sup> ]	2.10 (calcd.) <sup>[1]</sup>		
Heat of formation			
Heat of combustion			
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.

$-\Delta_{\text{ex}}U^{\circ} [\text{kJ kg}^{-1}]$		1,739 cal/cc (calcd.) <sup>[1,4]</sup>					
$T_{\text{ex}} [\text{K}]$							
$p_{\text{CJ}} [\text{kbar}]$		25.4 GPa (calcd.) <sup>[1,4]</sup>	23.3 GPa ( $\rho$ not specified, performance rate stick (plate dent)) <sup>[1]</sup> 23.3 GPa ( $\rho$ not specified) <sup>[4]</sup>				
VoD [ $\text{m s}^{-1}$ ]			7,850 ( $\rho$ not specified, performance rate stick (plate dent)) <sup>[1]</sup> 7,850 ( $\rho$ not specified, fiber optic) <sup>[4]</sup>				
$V_0 [\text{L kg}^{-1}]$							
Gap test	Similar shock sensitivity to Comp. B <sup>[2]</sup>						
Vacuum stability test [ $\text{cm}^3/\text{h}$ ]	Stable in vacuum @ 120 °C <sup>[3]</sup>						
Solubility [g/mL]	Soluble in acidic water <sup>[1]</sup> , soluble in acetonitrile <sup>[3]</sup> , recryst. from isopropanol <sup>[3]</sup> , soluble in water <sup>[4]</sup>						
Compatibility	Compatibility evaluations (1:1 mass:mass physical mixtures), DSC @ 5 °C/min, negative deviations $\geq 10$ °C indicate fail <sup>[1,4]</sup> :						
Compound	Pure compounds			Mixture with DNMT			
	mpt. (°C)	Exo onset (°C)	Exo max (°C)	mpt. (°C)	Exo onset (°C)	Exo max (°C)	
	DNMT	95.7	260.6	280.0			
	RDX	203.6	205.8	227.9	88.2	204.3	230.9
	HMX	187.2	276.3	284.2	93.7	223.4	252.8
	NTO	—	262.3	273.4	97.7	176.9	231.4
	TATB	—	366.56	373.8	97.6	227.1	243.5
	DNAN	94.2	326.9	342.9	54.8	301.6	322.3
	NQ	—	195.2	202.8	95.3	182.7	222.8
	DNP	86.5	275.8	296.9	46.25	285.4	345.6
DNTF	107.5	230.2	270.7	81.1/92.5	233.8	268.7	
Compatible with RDX, DNAN, DNP, DNTF <sup>[4]</sup>							
Environmental compatibility	No known environmental hazards <sup>[2]</sup>						

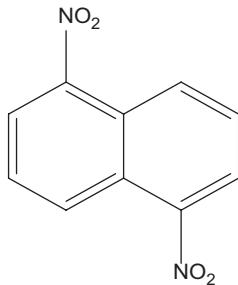
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## 1,5-Dinitronaphthalene

Name [German, acronym]: 1,5-Dinitronaphthalene,  $\alpha$ -dinitronaphthalene, alpha-dinitronaphthalene [1,5-dinitronaphthalin, 1,5-DNN]\*

Main (potential) use: Mixture of isomers as fuel in schneiderites<sup>[1]</sup>, isomer mixture is used in compositions for military and mining explosives – commonly referred to as dinol<sup>[11]</sup>, in ballistic powders<sup>[13]</sup>

Structural formula:



\* Commercial dinitronaphthalene is a mixture of the 1,5- and 1,8-isomers<sup>[12]</sup>.

	<b>1,5-Dinitronaphthalene</b>
Formula	$\text{C}_{10}\text{H}_6\text{N}_2\text{O}_4$
Molecular mass [g mol <sup>-1</sup> ]	218.17
Appearance at RT	Grayish-yellow crystals (any red color is due to $\text{NO}_2$ present) <sup>[11]</sup> , gray-yellow solid (commercial) <sup>[12]</sup> , yellow needle shaped crystals (monoclinic) <sup>[13]</sup>
IS [J]	11.01 <sup>[7]</sup> , 11.02 (Julius-Peters apparatus) <sup>[10,12]</sup>
ESD [J]	11.20 <sup>[5]</sup> , 180.0 <sup>[5]</sup> , 11.2 cal (calcd.) <sup>[12]</sup> , 13.91 cal (exptl.) <sup>[12]</sup> , 11.2 <sup>[17]</sup>
N [%]	12.84
$\Omega(\text{CO}_2)$ [%]	-139.3
$T_{\text{m.p.}}$ [°C]	216–217 <sup>[2]</sup> , 219 <sup>[8]</sup> , 217 <sup>[9,13]</sup> , 215–216 <sup>[11]</sup> , 216.5 <sup>[16]</sup>
$T_{\text{dec.}}$ [°C]	138 (isomer not specified, slow heating) <sup>[13]</sup> , >140 (commercial) <sup>[12]</sup>
$\rho$ [g cm <sup>-3</sup> ]	$1.481 \pm 0.06$ (@ 293.15 K) <sup>[3]</sup> , 1.602 (@ 18 °C) <sup>[8]</sup> , 1.578 (flootation method) <sup>[9]</sup> , 1.595 (crystals, flotation in benzene and $\text{CH}_2\text{I}_2$ ) <sup>[2]</sup>
Heat of formation	18.1 kJ/mol (enthalpy of form.) <sup>[4]</sup> , 140.0 kJ/kg (enthalpy of form.) <sup>[1]</sup> , -61 cal/g ( $Q_f$ ) <sup>[8]</sup> , -5.44 kcal/mol <sup>[12]</sup> , 30.6 kJ/mol (enthalpy of form., exptl.) <sup>[14]</sup> , 18.1 kJ/mol (enthalpy of form., calcld., emp.) <sup>[14]</sup> , 12.2 kJ/mol (enthalpy of form., calcld., S-D method) <sup>[14]</sup> , $29.7 \pm 5.8$ kJ/mol ( $\Delta H_f^\circ$ , (c)) <sup>[15]</sup>

Heat of combustion	1,152.6 kcal/mol ( $Q_c^P$ ) <sup>[8]</sup> , 1,152 kcal/mol (@ C) <sup>[11]</sup>	
	Lit. values	Exptl.
$-\Delta_{ex}U^\circ$ [kJ kg <sup>-1</sup> ]	3.075 kJ/mol (heat of det., calcd.) <sup>[12]</sup>	3,031 [H <sub>2</sub> O (l)] <sup>[1,6]</sup> 3,031 kJ/mol (heat of det.) <sup>[12]</sup>
$T_{ex}$ [K]		
$p_{C_J}$ [GPa]		13.00 GPa <sup>[12]</sup>
VoD [m s <sup>-1</sup> ]		~5,100 (highest VoD achieved when using a very powerful detonator; very difficult to detonate) <sup>[11]</sup> 1,150 (@ 1 g cm <sup>-3</sup> , isomer not specified) <sup>[13]</sup>
$V_0$ [L kg <sup>-1</sup> ]		488 <sup>[1]</sup>

Trauzl test [cm <sup>3</sup> , % TNT]	100 cc (DNN isomer not specified) <sup>[13]</sup>
Hess brisance	4 mm @ 0.9 g cm <sup>-3</sup> , with No. 8 detonating cap (DNN isomer not specified) <sup>[13]</sup>
5 s explosion $T$ [°C] Deflagration $T$ [°C] Ignition $T$ [°C] Detonation $T$ [°C]	318 (commercial) <sup>[12]</sup> 245 (dinitronaphthalene, heated wire) <sup>[13]</sup> 300–310 (DNN isomer not specified) <sup>[13]</sup>
Solubility [g/mL]	Sparingly soluble in EtOH and Et <sub>2</sub> O <sup>[11]</sup> , more soluble in benzene, toluene, acetic acid and acetone <sup>[11]</sup> Solubility (%): 0.16 in EtOH @ 22 °C <sup>[11]</sup> , 0.06 in EtOH (95%) @ 19 °C <sup>[11]</sup> , 0.59 in acetone @ 19 °C <sup>[11]</sup> , 2.3 in acetone @ boiling point <sup>[11]</sup> , 0.43 in acetic acid @ boiling point <sup>[11]</sup> , 2.01 in CHCl <sub>3</sub> @ 19 °C <sup>[11]</sup> , 0.45 in dichloroethane @ 19 °C <sup>[11]</sup> , 0.02 in benzene @ 50 °C <sup>[11]</sup> , insoluble in H <sub>2</sub> O @ boiling point <sup>[11]</sup> Commercial dinitronaphthalene is soluble in acetone, benzene and xylene <sup>[12]</sup>

	Solubility data from ref. <sup>[13]</sup> :		
Solvent	<i>T</i> of soln. (°C)	1,5-DNN	
Dichloroethane	19	0.45	
65% HNO <sub>3</sub>	19	0.01	
CHCl <sub>3</sub>	19	2.01	
Acetone	19	0.59	
Acetone	Boiling	2.3	
Benzene	19	0.5	
Benzene	Boiling	3.88	
Acetic acid	Boiling	0.43	
CS <sub>2</sub>	Boiling	Insoluble	
Abs. ethyl alcohol	22	0.16	
Gasoline	50	0.02	
Water	Boiling	Insoluble	
Pyridine	20	0.8	
Pyridine	Boiling	9.1	
5.800E-02 g/L in H <sub>2</sub> O @ 12 °C <sup>[16]</sup> .			

	1-5-DNN <sup>[9]</sup>	1-5-DNN <sup>[2]</sup>
Chemical formula	C <sub>10</sub> H <sub>6</sub> N <sub>2</sub> O <sub>4</sub>	C <sub>10</sub> H <sub>6</sub> N <sub>2</sub> O <sub>4</sub>
Molecular weight [g mol <sup>-1</sup> ]	218.2	218.2
Crystal system	Monoclinic	Monoclinic
Space group	<i>P</i> 2 <sub>1</sub> / <i>a</i>	
<i>a</i> [Å]	7.76 ± 0.02	7.85
<i>b</i> [Å]	16.32 ± 0.04	16.26
<i>c</i> [Å]	3.70 ± 0.01	3.70
α [°]	90	90
β [°]	101.48 ± 10	105.5
γ [°]	90	90
<i>V</i> [Å <sup>3</sup> ]	458.7	
<i>Z</i>	2	2
ρ <sub>calc</sub> [g cm <sup>-3</sup> ]	1.579	1.592
<i>T</i> [K]		

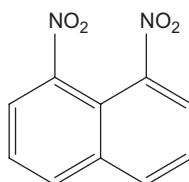
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## 1,8-Dinitronaphthalene

Name [German, acronym]: 1,8-Dinitronaphthalene,  $\beta$ -dinitronaphthalene, beta-dinitronaphthalene, peri-dinitronaphthalene  
[1,8-dinitronaphthalin, 1,8-DNN]\*

Main (potential) use: Mixture of isomers as fuel in schneiderites<sup>[1]</sup>, isomer mixture is used in compositions for military and mining explosives – commonly referred to as dinol<sup>[12]</sup>, in ballistic powders<sup>[14]</sup>

Structural formula:



\*Commercial dinitronaphthalene is a mixture of the 1,5- and 1,8-isomers<sup>[12]</sup>

	<b>1,8-DNN</b>
Formula	C <sub>10</sub> H <sub>6</sub> N <sub>2</sub> O <sub>4</sub>
Molecular mass [g mol <sup>-1</sup> ]	218.17
Appearance at RT	Grayish-yellow crystals (any red color is due to presence of NO <sub>2</sub> ) <sup>[12]</sup> , gray-yellow solid (commercial) <sup>[13]</sup> , yellow rhombic platelet crystals <sup>[14]</sup>
IS [J]	18.37 <sup>[8]</sup> , 18.37 (Julius-Peters apparatus) <sup>[9,13]</sup>
ESD [J]	13.99 <sup>[5,8]</sup> , 238.2 mJ <sup>[5]</sup> , 13.9 <sup>[6,17]</sup>
N [%]	12.84
$\Omega(\text{CO}_2)$ [%]	-139.3
T <sub>m.p.</sub> [°C]	171 <sup>[2]</sup> , 172.5–173 <sup>[10]</sup> , 170–172 <sup>[12]</sup> , >140 (commercial) <sup>[13]</sup> , 173.5 <sup>[14]</sup>
T <sub>phase transitions</sub> [°C]	Values from ref. <sup>[11]</sup> <div style="text-align: center;"> </div>

$T_{\text{dec.}} [^{\circ}\text{C}]$	318 (isomer not specified, slow heating) <sup>[14]</sup>	
$\rho [\text{g cm}^{-3}]$	$1.481 \pm 0.06$ (@ 293.15 K) <sup>[3]</sup> , 1.575 (@ 18 °C) <sup>[10]</sup>	
Heat of formation	37.6 kJ/mol (enthalpy of form., exptl.) <sup>[4]</sup> , 18.1 kJ/mol (enthalpy of form., calcd., emp.) <sup>[4]</sup> , 60.8 kJ/mol (enthalpy of form., calcd., S-D method) <sup>[4]</sup> , -60 cal/g ( $Q_f$ ) <sup>[10]</sup> , -2.65 kcal/mol <sup>[12]</sup> , $39.7 \pm 6.5$ kJ/mol ( $\Delta_f H^\circ$ , (c)) <sup>[16]</sup>	
Heat of combustion	1,164.5 kcal/mol ( $Q_c V$ ) <sup>[10]</sup> , 1,154 kcal/mol (@ C <sup>V</sup> ) <sup>[12]</sup>	
	Lit. values	Exptl.
$-\Delta_{\text{ex}} U^\circ [\text{kJ kg}^{-1}]$	3.075 kJ/mol (heat of det., calcd.) <sup>[13]</sup>	3,064 [H <sub>2</sub> O (l)] <sup>[1,7]</sup> 3,064 kJ/mol (heat of det.) <sup>[13]</sup>
$T_{\text{ex}} [\text{K}]$		
$p_{\text{CJ}} [\text{GPa}]$		13.10 GPa <sup>[13]</sup>
VoD [ $\text{m s}^{-1}$ ]		~5,100 (highest VoD achieved when using a very powerful detonator; very difficult to detonate) <sup>[12]</sup> 1,150 (@ 1 g cm <sup>-3</sup> , isomer not specified) <sup>[14]</sup>
$V_0 [\text{L kg}^{-1}]$		488 <sup>[1]</sup>

Trauzl test [cm <sup>3</sup> , % TNT]	100 cc (DNN isomer not specified) <sup>[14]</sup>
Hess brisance	4 mm @ 0.9 g cm <sup>-3</sup> , with No. 8 detonating cap (DNN isomer not specified) <sup>[14]</sup>
5 s explosion $T$ [°C] Explosion $T$ [°C] Deflagration $T$ [°C] Ignition $T$ [°C] Detonation $T$ [°C]	445 <sup>[10]</sup> 318 (commercial) <sup>[13]</sup> 245 (dinitronaphthalene, hot wire) <sup>[14]</sup> 300–310 (DNN isomer not specified) <sup>[14]</sup>
Solubility [g/mL]	Sparingly soluble in EtOH and Et <sub>2</sub> O <sup>[12]</sup> , more soluble in benzene, toluene, acetic acid and acetone <sup>[12]</sup> Solubility (%): 0.37 in EtOH @ 22 °C <sup>[12]</sup> , 0.06 in EtOH (95%) @ 19 °C <sup>[12]</sup> , 6.59 in acetone @ 19 °C <sup>[12]</sup> , 15.98 in acetone @ boiling point <sup>[12]</sup> , 2.01 in acetic acid @ boiling point <sup>[12]</sup> , 1.37 in CHCl <sub>3</sub> @ 19 °C <sup>[12]</sup> , 2.08 in dichloroethane @ 19 °C <sup>[12]</sup> , 0.06 in benzene @ 50 °C <sup>[12]</sup> , 0.07 in H <sub>2</sub> O @ boiling point <sup>[12]</sup> Commercial dinitronaphthalene is soluble in acetone, benzene and xylene <sup>[13]</sup>

	Solubility data from ref. <sup>[14]</sup> :		
Solvent	<i>T</i> of soln. (°C)	1,8-DNN	
Dichloroethane	19	2.08	
65% HNO <sub>3</sub>	19	0.02	
CHCl <sub>3</sub>	19	1.37	
Acetone	19	6.59	
Acetone	Boiling	13.98	
Benzene	19	2.01	
Benzene	Boiling	7.44	
Acetic acid	Boiling	2.01	
CS <sub>2</sub>	Boiling	—	
Abs. ethyl alcohol	22	0.37	
Gasoline	50	0.04	
Water	Boiling	0.07	
Pyridine	20	—	
Pyridine	Boiling	—	
3.400E-02 g/L in H <sub>2</sub> O @ 15 °C <sup>[15]</sup> .			

	1-8-DNN <sup>[11]</sup> (Phase I)	1-8-DNN <sup>[11]</sup> (Phase I)
Chemical formula	C <sub>10</sub> H <sub>6</sub> N <sub>2</sub> O <sub>4</sub>	C <sub>10</sub> H <sub>6</sub> N <sub>2</sub> O <sub>4</sub>
Molecular weight [g mol <sup>-1</sup> ]	218.2	218.2
Crystal system	Orthorhombic	Orthorhombic
Space group	<i>P</i> 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub> (no. 19)	<i>P</i> 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub> (no. 19)
<i>a</i> [Å]	11.375(1)	11.475(1)
<i>b</i> [Å]	14.974(5)	15.002(1)
<i>c</i> [Å]	5.388(1)	5.425(6)
α [°]	90	90
β [°]	90	90
γ [°]	90	90
<i>V</i> [Å <sup>3</sup> ]	917.734	933.903
<i>Z</i>	4	4
<i>ρ</i> <sub>calc</sub> [g cm <sup>-3</sup> ]	1.584	1.557
<i>T</i> [K]	22 °C	97 °C

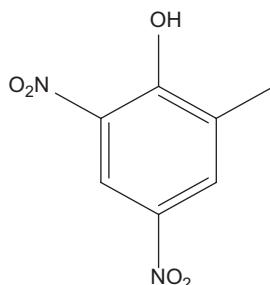
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## Dinitroorthocresol

Name [German, acronym]: Dinitroorthocresol, 4,6-dinitro-*o*-cresol  
[dinitro-*o*-kresol, DNCr]

Main (potential) use: Gelatinizer of nitrocellulose<sup>[1]</sup>

Structural formula:



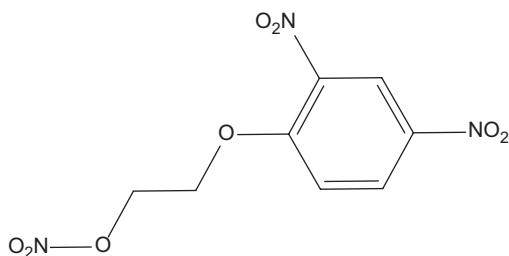
	<b>Dinitroorthocresol</b>	
Formula	C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> O <sub>5</sub>	
Molecular mass [g mol <sup>-1</sup> ]	198.13	
Appearance at RT		
IS [J]	>50 Nm <sup>[1]</sup>	
FS [N]	>353 <sup>[1]</sup>	
N [%]	14.14	
Ω(CO <sub>2</sub> ) [%]	-96.9	
T <sub>m.p.</sub> [°C]	86 <sup>[2]</sup>	
ρ [g cm <sup>-3</sup> ]	1.486 <sup>[1]</sup> , 1.550 ± 0.06 (@ 293.15 K) <sup>[3]</sup>	
Heat of formation	-254.4 kJ/mol ( $\Delta_f H^\circ$ ) <sup>[4]</sup> , -1,284.0 kJ/kg ( $\Delta_f H^\circ$ ) <sup>[4]</sup> , -1,009.4 kJ/kg ( $\Delta_f H^\circ$ ) <sup>[1]</sup>	
	Calcd. (EXPLO5 6.03)	Exptl.
-Δ <sub>ex</sub> U <sup>0</sup> [kJ kg <sup>-1</sup> ]	3,394	3,027 [H <sub>2</sub> O (l)] <sup>[1,5]</sup>
T <sub>ex</sub> [K]	2,606	
p <sub>C-J</sub> [GPa]	15.4	

VoD [ $\text{m s}^{-1}$ ]	6,144 (@ TMD)	
$V_0$ [ $\text{L kg}^{-1}$ ]	625	832 (calcd. or exptl. not specified) <sup>[1]</sup>

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## Dinitrophenoxyethylnitrate

Name [German, Acronym]: Dinitrophenoxyethylnitrate,  
 2-(2,4-dinitrophenoxy)ethyl nitrate  
 [dinitrophenylglykolethernitrat, DNPN]  
 Main (potential) use: Nitrocellulose gelatinizer<sup>[1]</sup>  
 Structural formula:



	<b>Dinitrophenoxyethylnitrate</b>		
Formula	C <sub>8</sub> H <sub>7</sub> N <sub>3</sub> O <sub>8</sub>		
Molecular mass [g mol <sup>-1</sup> ]	273.16		
Appearance at RT	Solid @ 298 K <sup>[8]</sup>		
IS [J]	20 Nm <sup>[1]</sup>		
N [%]	15.38		
Ω(CO <sub>2</sub> ) [%]	-67.4		
T <sub>m.p.</sub> [°C]	69 <sup>[2]</sup>		
ρ [g cm <sup>-3</sup> ]	1.60 <sup>[1]</sup> , 1.581 ± 0.06 (@ 293.15 K) <sup>[3]</sup>		
Heat of formation	-287.2 kJ/mol ( $\Delta_f H^\circ$ ) <sup>[4]</sup> , -1,051.4 kJ/kg ( $\Delta_f H^\circ$ ) <sup>[4]</sup> , -1,072.2 kJ/kg ( $\Delta_f H^\circ$ ) <sup>[1]</sup> , -298.8 kJ/mol (enthalpy of form., exptl.) <sup>[8]</sup> , -277.9 kJ/mol (enthalpy of form., calcd., emp.) <sup>[8]</sup> , -287.2 kJ/mol (enthalpy of form., calcd., S-D method) <sup>[8]</sup>		
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
-Δ <sub>ex</sub> U <sup>0</sup> [kJ kg <sup>-1</sup> ]	4,281		
T <sub>ex</sub> [K]	3,152		

$p_{\text{CJ}}$ [GPa]	18.3		
VoD [ $\text{m s}^{-1}$ ]	6,717 (@ TMD)	6,490 (@ 1.60 $\text{g cm}^{-3}$ (TMD), calcd., R-P method) <sup>[6]</sup>	6,800 (@ 1.58 $\text{g cm}^{-3}$ , confined) <sup>[1]</sup> 6,800 (@ 1.60 $\text{g cm}^{-3}$ ) <sup>[5]</sup>
$V_0$ [ $\text{L kg}^{-1}$ ]	673		

Trauzl test [ $\text{cm}^2$ , % TNT]	280 $\text{cm}^2$ <sup>[7]</sup>
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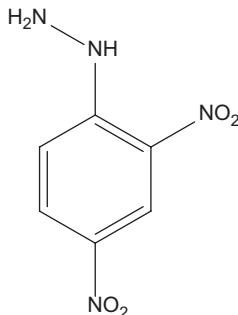
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## Dinitrophenylhydrazine

Name [German, acronym]: Dinitrophenylhydrazine [dinitrophenylhydrazin]

Main (potential) use: Preparation of dinitrophenylhydrazone and its derivatives from ketones and aldehydes<sup>[1]</sup>

Structural formula:



<b>Dinitrophenylhydrazine</b>		
Formula	$\text{C}_6\text{H}_6\text{N}_4\text{O}_4$	
Molecular mass [g mol <sup>-1</sup> ]	198.14	
Appearance at RT		
N [%]	28.28	
$\Omega(\text{CO}_2)$ [%]	-88.8	
$T_{\text{m.p.}}$ [°C]	197.94 <sup>[2]</sup>	
$T_{\text{dec.}}$ [°C]	202.25 (DSC @ 10 °C/min) <sup>[2]</sup>	
$\rho$ [g cm <sup>-3</sup> ]	$1.654 \pm 0.06$ (@ 293.15 K) <sup>[3]</sup> , 1.659 (X-ray @ 295 K) <sup>[6]</sup> , 1.705 (X-ray @ 120 K) <sup>[7]</sup>	
Heat of formation	46.7 kJ/mol ( $\Delta_f H^\circ$ ) <sup>[4]</sup> , 235.7 kJ/kg ( $\Delta_f H^\circ$ ) <sup>[4]</sup> , 252.1 kJ/kg (enthalpy of form.) <sup>[1]</sup> , 9.2 kcal/mol (@ constant pressure) <sup>[5]</sup>	
Heat of combustion	3,950 cal/g (@ constant pressure) <sup>[5]</sup>	
	Calcd. (EXPLO5 6.03)	Exptl.
$-\Delta_{\text{ex}} U^\circ$ [kJ kg <sup>-1</sup> ]	3,962	
$T_{\text{ex}}$ [K]	2,813	

$p_{\text{CJ}}$ [GPa]	17.9	
VoD [ $\text{m s}^{-1}$ ]	6,892 (@ TMD)	
$V_0$ [ $\text{L kg}^{-1}$ ]	686	

	Dinitrophenylhydrazine <sup>[6]</sup>	Dinitrophenylhydrazine <sup>[7]</sup>
Chemical formula	$\text{C}_6\text{H}_6\text{N}_4\text{O}_4$	$\text{C}_6\text{H}_6\text{N}_4\text{O}_4$
Molecular weight [g mol <sup>-1</sup> ]	198.14	198.14
Crystal system	Monoclinic	Monoclinic
Space group	$P2_1/c$ (no. 14)	$P2_1/c$ (no. 14)
$a$ [\mathring{A}]	4.819(3)	4.7917(2)
$b$ [\mathring{A}]	11.625(4)	11.5905(6)
$c$ [\mathring{A}]	14.268(4)	14.0496(5)
$\alpha$ [°]	90	90
$\beta$ [°]	97.04(4)	98.372(3)
$\gamma$ [°]	90	90
$V$ [\mathring{A} <sup>3</sup> ]	739.28	771.97(6)
$Z$	4	4
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.659	1.705
$T$ [K]	295	120

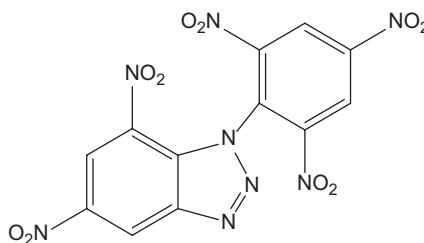
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## 5,7-Dinitro-1-picrylbenzotriazole

Name [German, acronym]: 1-(2',4',6'-Trinitrophenyl)-5,7-dinitrobenzotriazole  
[5,7-dinitro-1-picrylbenzotriazol, BTX]

Main (potential) use: Thermally stable detonator explosive<sup>[1]</sup>, described as high-temperature resistant exploding bridgewire<sup>[4]</sup>

Structural formula:



	<b>BTX</b>
Formula	C <sub>12</sub> H <sub>4</sub> N <sub>8</sub> O <sub>10</sub>
Molecular mass [g mol <sup>-1</sup> ]	420.21
Appearance at RT	Slightly yellow crystals <sup>[2]</sup> , large platelet crystals of <100 m <sup>2</sup> /kg specific surface (crude BTX) <sup>[4]</sup> , pale yellow solid <sup>[5]</sup>
IS [J]	33 cm <sup>[1]</sup> , 350 mm (type 12) <sup>[4]</sup> , 330 mm (type 12 B) <sup>[4]</sup> , F of I = 30 (cf. RDX = 80, Rotter impact test, 5 kg mass, metal cup, 30 mg sample) <sup>[2,5]</sup> , H <sub>50%</sub> = 27 cm, 35 cm (35 mg sample as conical pile on sand paper, 2.5 kg mass, B.M. apparatus, cf. RDX = 25 cm) <sup>[2]</sup>
FS [N]	Negative at all angles <sup>[4]</sup>
ESD [J]	0.48 (76 µm foil) <sup>[4]</sup> , ignites @ 4.5 J but not at 0.45 J (ERDE electric spark test, loose powder) <sup>[5]</sup> , 6.5 <sup>[7]</sup>
N [%]	26.67
Ω(CO <sub>2</sub> ) [%]	-60.9
T <sub>m.p.</sub> [°C]	263 <sup>[1,5,6]</sup> , 258 (crystal) <sup>[2]</sup> , 263 (DTA @ 20 °C/min) <sup>[4]</sup> , 258 (hot strip) <sup>[2,5]</sup> , 256 (DSC @ 20 K/min, Al pan with lid placed on sample) <sup>[2,5]</sup>
T <sub>dec.</sub> [°C]	Stable to mpt. (DTA @ 20 °C/min) <sup>[4]</sup> , 308 (DSC @ 20 K/min, Al pan with lid placed on sample) <sup>[2,5]</sup>
ρ [g cm <sup>-3</sup> ]	1.74 (crystal) <sup>[1,4]</sup> , 1.756 (X-ray) <sup>[2]</sup> , 1.74 (gas comparison pycnometer) <sup>[2,5]</sup> , 1.78 (calcd., Cichra et al.) <sup>[2]</sup> , 1.81 (est., empirical method) <sup>[5]</sup> , 1.74 <sup>[6]</sup>
Heat of formation	70.9 kcal/mol (ΔH <sub>f</sub> <sup>o</sup> ) <sup>[6]</sup>
Heat of combustion	ΔH <sub>c</sub> <sup>o</sup> = -1,336.2 kcal/mol <sup>[6]</sup>

	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^\circ [\text{kJ kg}^{-1}]$			
$T_{\text{ex}} [\text{K}]$			
$p_{\text{C-J}} [\text{kbar}]$		23.4 GPa <sup>[1]</sup>  23.2 GPa ( $\rho$ not specified, calcd., R-P method) <sup>[2]</sup>  23.4 GPa ( $\rho$ not specified, calcd.) <sup>[4]</sup>  23 GPa ( $\rho$ not specified, calcd.) <sup>[5]</sup>	
$\text{VoD} [\text{m s}^{-1}]$		7,170 ( $\rho$ not specified) <sup>[1]</sup>  7,370 ( $\rho$ not specified, calcd., R-P method) <sup>[2]</sup>  7,170 ( $\rho$ not specified, calcd.) <sup>[4]</sup>  7,370 ( $\rho$ not specified, calcd.) <sup>[5]</sup>	
$V_0 [\text{L kg}^{-1}]$			
$5 \text{ s explosion } T [\text{ }^\circ\text{C}]$ Ignition $T [\text{ }^\circ\text{C}]$	304 (ERDE test, 50 mg unconfined sample, heated a 5 °C/min in test tube, explosion) <sup>[5]</sup>		
Thermal stability	BTX powder heated to 175 °C for 50 h and then loaded into an SE-1 detonator: specific surface changed to 1,700 m <sup>2</sup> /kg and only a small effect was observed on detonator timing and on voltage threshold in comparison with the unheated BTX <sup>[4]</sup>		
Vacuum stability test [cm <sup>3</sup> /h]	@ 175 °C, total gas evolved (cm <sup>3</sup> /g) @ STP/time of exposure (days) <sup>[3,4]</sup> : 0.2/2, 0.3/7, 0.4/14, 0.4/21, 0.5/28, 0.6/35, 0.7/42, 0.8/49, 1.0/56, 1.1/63, 1.1/70, 1.2/77, 1.2/84, 1.3/91 <sup>[3,4]</sup> 1.0 mL/g, 48 h @ 200 °C <sup>[4]</sup> , 1.3 mL/g, 91 days @ 175 °C <sup>[4]</sup>		
Solubility [g/mL]	Soluble in acetone <sup>[4]</sup> , insoluble in water <sup>[4]</sup> , recryst. by addition of water to BTX/acetone soln. <sup>[4]</sup>		
Heat of dec [J/g]	152.6 kcal/mol (DSC @ 20 K/min, Al pan with lid placed on sample) <sup>[2,5]</sup>		
Heat of fusion [J/g]	9.6 kcal/mol (DSC @ 20 K/min, Al pan with lid placed on sample) <sup>[2,5]</sup>		

EBW initiation	Initial pressing $\rho$ of 0.90 g cm <sup>-3</sup> , 2.2 $\mu$ s transit time when two detonators fired in parallel at a 7.0 kV firing voltage, BTX specific surface ~ 2200 m <sup>2</sup> /kg (cf. 2.0 $\mu$ s for PETN) <sup>[4]</sup> , with 900 m <sup>2</sup> /kg specific surface detonator performance was poor <sup>[4]</sup> , all detonations failed with ~ 100 m <sup>2</sup> /kg specific surface platelet crystals <sup>[4]</sup> , bridgewire burst current at 7.0 kV = 7 kA and burst power = 15 MW (using two detonators in parallel and 130 $\mu$ m diameter by 1 mm long gold bridgewire) <sup>[4]</sup> , bridgewire length study: voltage threshold with 0.5 mm long bridge = 5.0 kV, 1 mm length = 3.0 kV, with 1.5 mm length initiation delay at the bridge was reduced for the firing voltages below 7.0 kV, although threshold remained at 3.0 kV, at 2.3 mm length no further improvement was seen <sup>[4]</sup>
Booster pellet initiation	Ability of a BTX initial pressing to initiate a high-density pellet: initiation of 1.60 g cm <sup>-3</sup> density BTX pellet was marginal <sup>[4]</sup> , staged pellet density arrangement performed acceptably in most tests <sup>[4]</sup> , initiation delay in 1.2 g cm <sup>-3</sup> pellet was ~0.2 $\mu$ s, but was small in the other pellets <sup>[4]</sup>
Plate dent test	Dent produced by BTX detonator (detonation pressure = 23.4 GPa) is a little smaller than that produced by PETN detonator (detonation pressure = 33 GPa) (6 mm thick Dural plate) <sup>[4]</sup>

<b>5,7-Dinitro-1-picrylbenzotriazole<sup>[2]</sup></b>	
Chemical formula	C <sub>12</sub> H <sub>4</sub> N <sub>8</sub> O <sub>10</sub>
Molecular weight [g mol <sup>-1</sup> ]	420.2
Crystal system	Monoclinic
Space group	P2 <sub>1</sub> /c (no. 14)
<i>a</i> [ $\text{\AA}$ ]	6.697(2)
<i>b</i> [ $\text{\AA}$ ]	20.325(5)
<i>c</i> [ $\text{\AA}$ ]	11.868(3)
$\alpha$ [°]	90
$\beta$ [°]	100.25(2)
$\gamma$ [°]	90
<i>V</i> [ $\text{\AA}^3$ ]	1,589.5(7)
<i>Z</i>	4
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.756
<i>T</i> [K]	295

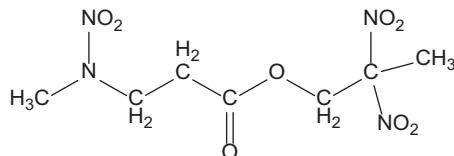
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- [6] *LASL Explosive Property Data*, T. R. Gibbs, A. Popolato (eds.), University of California Press, Berkeley, **1980**.
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## 2,3-Dinitropropyl-4-nitro-4-azapentanoate

Name [German, acronym]: 2,3-Dinitropropyl-4-nitro-4-azapentanoate  
 [2,3-dinitropropyl-4-nitro-4-azapentanoat, DNP-4-NAP]

Main (potential) use: Possible use as energetic plasticizer

Structural formula:



	DNP-4-NAP		
Formula	$C_7H_{12}N_4O_8$		
Molecular mass [g mol <sup>-1</sup> ]	280.19		
Appearance at RT	Pale yellow oil, crystallizes on standing @ 4 °C or on standing for several days <sup>[1]</sup>		
IS [J]	35 Nm (10 kg mass, 0.35 m drop-height, $\frac{3}{6}$ runs positive with weak bang, BAM) <sup>[1]</sup>		
FS [N]	96 (pistil load 9.6 kp, $\frac{2}{6}$ runs positive with flamelet, BAM) <sup>[1]</sup>		
N [%]	20.0		
$\Omega(CO_2)$ [%]	-68.52		
$T_{m.p.}$ [°C]	36–36 (after solidified on standing) (DSC @ 5 °C/min, Al pans, under Ar flux, 1058 J/g energy release) <sup>[1]</sup>		
$T_{\text{glass transition}}$ [°C]	-52.4 (DSC @ 5 °C/min, Al pans, under Ar flux) <sup>[1]</sup>		
$T_{\text{dec.}}$ [°C]	185–270 (exo peak) 249.41 (exo, peak max.) (DSC @ 5 °C/min, Al pans, under Ar flux) <sup>[1]</sup> , 185–270 (single step weight loss of 99.36%, TGA) <sup>[1]</sup>		
$\rho$ [g cm <sup>-3</sup> ]	1.397 <sup>[1]</sup>		
Heat of formation	-1,668.89 kJ/kg (enthalpy of formation) <sup>[1]</sup>		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^\circ$ [kJ kg <sup>-1</sup> ]			
$T_{\text{ex}}$ [K]			
$p_{\text{C-J}}$ [kbar]			

VoD [ $\text{m s}^{-1}$ ]			
$V_0$ [ $\text{L kg}^{-1}$ ]			
Vacuum stability test [ $\text{cm}^3/\text{h}$ ]	0.57 mL/g (vol. of evolved gas @ 100 °C within 40 h, max. limit for passing = 1.2–2.0 mg/g) <sup>[1]</sup>		
Refractive index	1.4899 (@ 20 °C) <sup>[1]</sup>		
Dutch test	0.25% weight loss within 8–72 h @ 105 °C (max. limit for passing = 2%) <sup>[1]</sup>		
$\Delta H_{\text{melt}}$ [J/g]	1058 (DSC @ 5 °C/min, Al pans, under Ar flux) <sup>[1]</sup>		

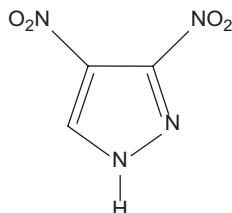
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## 3(5),4-Dinitropyrazole

Name [German, acronym]: 3,4-Dinitropyrazole [3,4-dinitropyrazol, DNP]

Main (potential) use: potential new melt-cast matrix<sup>[1]</sup>

Structural formula:



	DNP
Formula	C <sub>3</sub> H <sub>2</sub> N <sub>4</sub> O <sub>4</sub>
Molecular mass [g mol <sup>-1</sup> ]	158.07
Appearance at RT	Colorless block crystals <sup>[5]</sup>
IS [J]	$Ed_{min} = 20$ (BAM, 5 kg mass, RT) <sup>[1]</sup> , 55 cm <sup>[4]</sup> , 67.4 cm (ERL apparatus) <sup>[9]</sup> , Navy method: 54.1 cm (premelt), 146.9 cm (postmelt) <sup>[9]</sup>
FS [N]	$G_{min} = 360$ (BAM Julius-Peters, max level with 6 consec. negative runs) <sup>[1]</sup> , 246 <sup>[4]</sup> , >216 (BAM) <sup>[9]</sup>
ESD [J]	0.2625 <sup>[4]</sup> , >0.25 <sup>[9]</sup>
N [%]	35.44
$\Omega(\text{CO}_2)$ [%]	-30.4
$T_{\text{m.p.}}$ [°C]	89 (DSC, Al cup with pierced lid, N <sub>2</sub> atmosphere, very pure DNP evaporates on heating, crude DNP shows no evaporation) <sup>[1]</sup> , 86.48 (DSC @ 10 °C/min, hermetic pan, pinhole lid, under nitrogen) <sup>[2]</sup> , 88.83 (DSC @ 10 °C/min, standard pan, under nitrogen) <sup>[2]</sup> , 87 <sup>[4]</sup> , 360.65 K <sup>[5]</sup> , 85–87 (capillary method) <sup>[6]</sup> , 90–91 <sup>[6]</sup> , 87 (@ 1 bar) <sup>[7]</sup> , 87 (@ 50 bar) <sup>[7]</sup> , 363–364 K <sup>[8]</sup> , ~85 <sup>[9]</sup> , 86.54 (endo peak max, DSC @ 5 °C/min) <sup>[9]</sup>
$T_{\text{b.p.}}$ [K]	574.5 (est., $T_{\text{nbp}}$ ) <sup>[8]</sup>
$T_{\text{evaporation}}$ [°C]	180 (DSC, Al cup with pierced lid, N <sub>2</sub> atmosphere, very pure DNP, crude DNP shows no evaporation) <sup>[1]</sup>
$T_{\text{dec.}}$ [°C]	216 (DSC, Al cup with pierced lid, N <sub>2</sub> atmosphere, crude DNP, very pure DNP showed no dec. on heating) <sup>[1]</sup> , 297 (onset, TG @ 10 K/min) <sup>[7]</sup> , 306 (onset, $T_{\text{max}} = 338$ , 376 and 404 °C, DSC @ 10 K/min, closed alumina pans with pierced lids, dynamic Ar atmosphere) <sup>[7]</sup> , 310 (onset, $T_{\text{max}} = 346$ , 359 and 404 °C, DSC @ 10 K/min, @ 50 bar, Al crucibles covered with pierced lids, N <sub>2</sub> flow) <sup>[7]</sup> , 275.78 (exo, onset), 296.95 (exo peak max) (DSC @ 5 °C/min) <sup>[9]</sup>

$\rho$ [g cm <sup>-3</sup> ]	1.773 <sup>[4]</sup> , 1.81 ( $\rho$ bottle method) <sup>[6]</sup> , 1.87 (calcd.) <sup>[9]</sup> , 1.841 (X-ray @ 105 K) <sup>[5]</sup>		
Heat of formation	120.5 (no units given) <sup>[4]</sup>		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^{\circ}$ [kJ kg <sup>-1</sup> ]		1,961 cal/cc (calcd.) <sup>[9]</sup>	
$T_{\text{ex}}$ [K]		4,033 (@ 1.791 g cm <sup>-3</sup> , $\Delta H_f = 120.5$ kJ/mol, calcd., JAGUAR) <sup>[3]</sup>	
$p_{\text{CJ}}$ [kbar]		32.5 GPa (@ 1.776 g cm <sup>-3</sup> , $\Delta H_f = 185.2$ kJ/mol, calcd., CHEETAH) <sup>[1]</sup>  30.9 GPa (@ 1.791 g cm <sup>-3</sup> , $\Delta H_f = 120.5$ kJ/mol, calcd., JAGUAR) <sup>[3]</sup>  29.24 GPa (calcd., CHEETAH 7.0) <sup>[4]</sup>  28.8 GPa (calcd.) <sup>[9]</sup>	29.4 GPa (performance rate stick/plate dent) <sup>[9]</sup>
VoD [m s <sup>-1</sup> ]		8,516 (@ 1.776 g cm <sup>-3</sup> , $\Delta H_f = 185.2$ kJ/mol, calcd., CHEETAH) <sup>[1]</sup>  8,310 (@ 1.791 g cm <sup>-3</sup> , $\Delta H_f = 120.5$ kJ/mol, calcd., JAGUAR) <sup>[3]</sup>  8,160 (@ 1.75 g cm <sup>-3</sup> , calcd., JAGUAR) <sup>[25]</sup>  8,251 (@ 1.773 g cm <sup>-3</sup> , calcd., CHEETAH 7.0) <sup>[4]</sup>	8,100 (@ 1.75 g cm <sup>-3</sup> ) <sup>[3]</sup>  8,104 GPa ( $\rho$ not specified, performance rate stick/plate dent) <sup>[9]</sup>
$V_0$ [L kg <sup>-1</sup> ]			
Critical pressure [bar]	69.3 (est. Joback-Stein method) <sup>[8]</sup> , 59.72 (est., Valderrama-Alveraz method) <sup>[8]</sup>		
Critical $T$ [K]	816.8 (est. Joback-Stein method) <sup>[8]</sup> , 1036.4 (est., Valderrama-Alveraz method) <sup>[8]</sup>		

Vapor pressure [atm @ °C]	$2.42 \times 10^{-11}$ Torr (@ 25 °C est.) <sup>[2,4]</sup> , $1.57 \times 10^{-8}$ Torr (@ 70 °C, est.) <sup>[2,4]</sup> , $2.72 \times 10^{-6}$ Torr (@ 100 °C, est.) <sup>[2,4]</sup>																																																																				
VTS	2.6803 cc (total gas evolved after 40 h @ 100 °C) <sup>[4]</sup>																																																																				
Solubility [g/mL]	6.7 × 10 <sup>-1</sup> mg/mL in H <sub>2</sub> O @ 23 °C <sup>[2]</sup> , 0.51 g/L in H <sub>2</sub> O @ 298.15 K (est. Klopman method) <sup>[8]</sup> , 0.733 g/L in H <sub>2</sub> O @ 298.15 K (est. COSMOtherm) <sup>[8]</sup>																																																																				
Compatibility	<p>VTS compatibility (STANAG 4147 test 1B, 2.5 g of compound 1 mixed with 2.5 g of compound 2, total gas evolved after 40 h @ 100 °C, values in cc)<sup>[4]</sup>: 2.6083 (neat), 2.0563 (DNGU), 1.6351 (LLM-105), 0.2971 (HK-56), – (HMX) concluding that DNGU, LLM-105, HK-56 and HMX are compatible with DNP<sup>[4]</sup></p> <p>Compatibility evaluations (1:1 mass:mass physical mixtures), DSC @ 5 °C/min, negative deviations ≥10 °C indicate fail<sup>[9]</sup>:</p> <table border="1"> <thead> <tr> <th rowspan="2">Compound</th> <th colspan="3">Pure compound</th> <th colspan="3">Mixture with DNP</th> </tr> <tr> <th>mpt. (°C)</th> <th>Exo onset (°C)</th> <th>Exo max (°C)</th> <th>mpt. (°C)</th> <th>Exo onset (°C)</th> <th>Exo max (°C)</th> </tr> </thead> <tbody> <tr> <td>DNP</td> <td>86.5</td> <td>275.8</td> <td>296.9</td> <td></td> <td></td> <td></td> </tr> <tr> <td>RDX</td> <td>203.6</td> <td>205.8</td> <td>227.9</td> <td>83.8</td> <td>202.6</td> <td>234</td> </tr> <tr> <td>HMX</td> <td>187.2</td> <td>276.3</td> <td>284.2</td> <td>86.7</td> <td>203.3</td> <td>221.2</td> </tr> <tr> <td>NTO</td> <td>–</td> <td>262.3</td> <td>273.4</td> <td>86.4</td> <td>175.7</td> <td>237.7</td> </tr> <tr> <td>TATB</td> <td>–</td> <td>366.56</td> <td>373.8</td> <td>86.7</td> <td>193.3</td> <td>273.7</td> </tr> <tr> <td>DNAN</td> <td>94.2</td> <td>326.9</td> <td>342.9</td> <td>57.9</td> <td>203.9</td> <td>302.9</td> </tr> <tr> <td>NQ</td> <td>–</td> <td>195.2</td> <td>202.8</td> <td>84.2</td> <td>182.5</td> <td>222.7</td> </tr> </tbody> </table>							Compound	Pure compound			Mixture with DNP			mpt. (°C)	Exo onset (°C)	Exo max (°C)	mpt. (°C)	Exo onset (°C)	Exo max (°C)	DNP	86.5	275.8	296.9				RDX	203.6	205.8	227.9	83.8	202.6	234	HMX	187.2	276.3	284.2	86.7	203.3	221.2	NTO	–	262.3	273.4	86.4	175.7	237.7	TATB	–	366.56	373.8	86.7	193.3	273.7	DNAN	94.2	326.9	342.9	57.9	203.9	302.9	NQ	–	195.2	202.8	84.2	182.5	222.7
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$\Delta H_{\text{vap}}$ [kJ/mol]	141.4 (est.) <sup>[2,4]</sup>																																																																				
$\Delta H_{\text{melt}}$ [J/g]	−104 ( $Q_m$ , @ 1 bar) <sup>[7]</sup> , −100 ( $Q_m$ @ 50 bar) <sup>[7]</sup> , 27.6 kJ/mol (est.) <sup>[8]</sup> , 120.6 (DSC) <sup>[9]</sup>																																																																				
$\Delta H_{\text{dec}}$ [J/g]	2,360 ( $Q_{\text{dec}}$ @ 1 bar) <sup>[7]</sup> , 3710 ( $Q_{\text{dec}}$ @ 50 bar) <sup>[7]</sup>																																																																				
$K_{\text{ow}}$	4.7 <sup>[2]</sup> , log $K_{\text{ow}} = 0.67$ <sup>[2]</sup> , 0.9 (est., Broto) <sup>[8]</sup> , −0.99 (est., Ghose) <sup>[8]</sup> , 0.27 (est., COSMOtherm) <sup>[8]</sup>																																																																				
$K_{\text{oc}}$	29.3 (measured) <sup>[2]</sup> , log $K_{\text{oc}} = 1.47$ <sup>[2]</sup> , 7.23 (predicted) <sup>[2]</sup>																																																																				
p $K_a$	$pK_{\text{BH}^+} = -8.06$ (@ 20 °C, in water, spectrophotometrically) <sup>[10]</sup>																																																																				

	<b>3,4-Dinitropyrazole<sup>[5]</sup></b>
Chemical formula	C <sub>3</sub> H <sub>2</sub> N <sub>4</sub> O <sub>4</sub>
Molecular weight [g mol <sup>−1</sup> ]	158.09
Crystal system	Monoclinic
Space group	P2 <sub>1</sub> /c (no. 14)

$a$ [Å]	9.7013(13)
$b$ [Å]	12.0797(10)
$c$ [Å]	9.7587(7)
$\alpha$ [°]	90
$\beta$ [°]	93.962(11)
$\gamma$ [°]	90
$V$ [Å <sup>3</sup> ]	1,140.88(19)
$Z$	8
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.841
$T$ [K]	105.3

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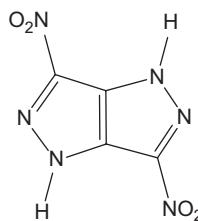
## 3,6-Dinitropyrazolo[4,3-c]pyrazole

Name [German, acronym]: 3,6-Dinitropyrazolo[4,3-c]pyrazole

[3,6-dinitropyrazolo[4,3-c]pyrazol, DNPP]

Main (potential) use: Potential new explosive ingredient<sup>[2]</sup>, precursor for synthesis of LLM-119<sup>[2,6]</sup>

Structural formula:



	DNPP		
Formula	C <sub>4</sub> H <sub>2</sub> N <sub>6</sub> O <sub>4</sub>		
Molecular mass [g mol <sup>-1</sup> ]	198.10		
Appearance at RT			
IS [J]	DH <sub>50</sub> = 68 cm (5 kg mass) <sup>[1,2,5]</sup> , 15 (BAM) <sup>[5]</sup> , 15 <sup>[6]</sup>		
FS [N]	Not sensitive <sup>[2]</sup> , 160 (BAM) <sup>[5]</sup> , 160 <sup>[6]</sup>		
ESD [J]	Not sensitive <sup>[2]</sup>		
N [%]	42.42		
Ω(CO <sub>2</sub> ) [%]	-40.4		
T <sub>m.p.</sub> [°C]			
T <sub>dec.</sub> [°C]	330 (exo, DSC) <sup>[1,2,5]</sup> , 603 K (exotherm, DSC) <sup>[4]</sup> , 336 (DSC @ 5 °C/min) <sup>[5]</sup> , 336 (onset) <sup>[6]</sup>		
ρ [g cm <sup>-3</sup> ]	1.865 (crystal) <sup>[1,2]</sup> , 2.0 (calcd., MOLPAK) <sup>[4]</sup> , 1.9 (calcd. group additivity method) <sup>[4]</sup> , 1.865 (X-ray) <sup>[4,5]</sup> , 1.85 (gas pycnometry) <sup>[5,6]</sup>		
Heat of formation	65 kcal/mol (Δ <sub>f</sub> H, exptl.) <sup>[1,2]</sup> , 272 kJ/mol (ΔH <sub>f</sub> , measured) <sup>[4]</sup> , 339 kJ/mol (corrected HF calcd.) <sup>[4]</sup> , 287 kJ/mol (DFT calcd.) <sup>[4]</sup> , 323 kJ/mol (ΔH <sub>f</sub> , calcd.) <sup>[5]</sup> , 322.6 kJ/mol (ΔH <sub>f</sub> , heat of form.) <sup>[6]</sup>		
	Calcd. (EXPLO5 6.01)	Lit. values	Exptl.
-Δ <sub>ex</sub> U <sup>0</sup> [kJ kg <sup>-1</sup> ]			
T <sub>ex</sub> [K]			

$p_{\text{CJ}}$ [kbar]	27.4 GPa (@ 1.85 g cm <sup>-3</sup> ) <sup>[6]</sup>	27.4 GPa (@ 1.85 g cm <sup>-3</sup> , calcd) <sup>[5]</sup>	
VoD [m s <sup>-1</sup> ]	8250 (@ 1.85 g cm <sup>-3</sup> ) <sup>[6]</sup>	8250 (@ 1.85 g cm <sup>-3</sup> , calcd., K-J) <sup>[5]</sup>	
$V_0$ [L kg <sup>-1</sup> ]			
$I_{\text{sp}}$ [s]	241 <sup>[6]</sup>		
$p_{\text{k}_a}$	6 and 3 (dibasic acid) <sup>[4]</sup>		

	<b>DNPP•H<sub>2</sub>O<sup>[3]</sup></b>	<b>DNPP•2H<sub>2</sub>O<sup>[5]</sup></b>
Chemical formula	C <sub>4</sub> H <sub>4</sub> N <sub>6</sub> O <sub>5</sub>	C <sub>4</sub> H <sub>6</sub> N <sub>6</sub> O <sub>6</sub>
Molecular weight [g mol <sup>-1</sup> ]	216.15	234.15
Crystal system	Monoclinic	Triclinic
Space group	<i>P</i> 2 <sub>1</sub> / <i>c</i>	<i>P</i> -1
<i>a</i> [\AA]	3.480(4)	5.0574(14)
<i>b</i> [\AA]	14.134(16)	9.395(3)
<i>c</i> [\AA]	9.027(11)	9.872(3)
$\alpha$ [°]	90	100.110(4)
$\beta$ [°]	94.327(16)	97.281(4)
$\gamma$ [°]	90	100.102(4)
<i>V</i> [\AA <sup>3</sup> ]	442.7(9)	
<i>Z</i>	4	2
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.756	1.734
<i>T</i> [K]		296

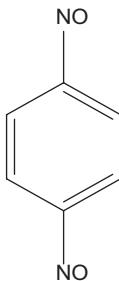
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## Dinitrosobenzene

Name [German, acronym]: Dinitrosobenzene [dinitrosobenzol]

Main (potential) use: unknown

Structural formula:



	Dinitrosobenzene	
Formula	C <sub>6</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub>	
Molecular mass [g mol <sup>-1</sup> ]	136.11	
Appearance at RT		
IS [J]	15 Nm <sup>[1]</sup>	
FS [N]	>353 <sup>[1]</sup>	
N [%]	20.58	
Ω(CO <sub>2</sub> ) [%]	-141.1	
T <sub>m.p.</sub> [°C]	Dec. <sup>[1]</sup>	
T <sub>dec.</sub> [°C]	184 (onset of brown discoloration) <sup>[4]</sup>	
ρ [g cm <sup>-3</sup> ]	1.30 ± 0.1 (@ 293.15 K) <sup>[2]</sup>	
Heat of formation		
	Calcd. (K-J)	Exptl.
-Δ <sub>ex</sub> U° [kJ kg <sup>-1</sup> ]		
T <sub>ex</sub> [K]		
p <sub>C-J</sub> [GPa]		
VoD [m s <sup>-1</sup> ]		
V <sub>0</sub> [L kg <sup>-1</sup> ]		

	<i>ortho</i> -Dinitrosobenzene <sup>[3]*</sup>
Chemical formula	C <sub>6</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub>
Molecular weight [g mol <sup>-1</sup> ]	136.11
Crystal system	Triclinic
Space group	P-1 (no. 2)
a [Å]	7.50
b [Å]	7.70
c [Å]	6.71
α [°]	114.67
β [°]	112.50
γ [°]	99.40
V [Å <sup>3</sup> ]	300.28
Z	2
ρ <sub>calc</sub> [g cm <sup>-3</sup> ]	1.505
T [K]	295

\*Note this structure is for the ortho and not the para isomer. Values given in the other tables are for the para isomer.

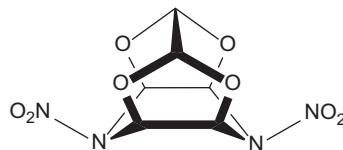
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## 4,10-Dinitro-2,6,8,12-tetraoxa-4,10-diazaisowurtzitane

Name [German, acronym]: 4,10-Dinitro-2,6,8,12-tetraoxa-4,10-diazaisowurtzitane, 4,10-dinitro-2,6,8,12-tetraoxa-4,10-diazatetracyclo[5.5.0.0<sup>3,11</sup>]dodecane, dinitrotetraoxadiazaisowurzitane [4,10-dinitro-2,6,8,12-tetraoxa-4,10-diazaisowurtzitan, TEX, DTIW, TOIW, DNITD]

Main (potential) use: Very insensitive high explosive<sup>[1]</sup>, promising insensitive explosive<sup>[19]</sup>

Structural formula:



	TEX
Formula	C <sub>6</sub> H <sub>6</sub> N <sub>4</sub> O <sub>8</sub>
Molecular mass [g mol <sup>-1</sup> ]	262.13
Appearance at RT	Colorless crystals <sup>[19]</sup>
IS [J]	23 <sup>[2,7,8]</sup> , 5.10 (first reaction) <sup>[4,13]</sup> , 24.25 (sound) <sup>[4,13]</sup> , 15–19 Nm <sup>[1]</sup> , >23–25 <sup>[15]</sup> , H <sub>50</sub> ≥ 177 cm (2 kg mass) <sup>[14]</sup> , H <sub>50</sub> = 50 cm (5 kg hammer) <sup>[10,19]</sup> , H <sub>50%</sub> ≥ 46 in (200 µm, Thiokol) <sup>[12]</sup> , 33 cm (200 µm, ABL) <sup>[12,19]</sup> , E <sub>dmin</sub> = 15 J (5/5 negative results) – 22.5 J (1/5 positive tests) <sup>[8]</sup> , H <sub>50</sub> = 45.5 cm (23 J, 5 kg hammer) <sup>[8]</sup> , A <sub>d1</sub> = 32%, A <sub>d2</sub> = 40%, LL = 1.2 m, A <sub>50 d1</sub> = 2.5 m, A <sub>50 d2</sub> = 2.8 <sup>[18]</sup> , no go 23–25 <sup>[19]</sup> , >116.8 cm (Thiokol/ATK impact hammer) <sup>[19]</sup> , 42.5 cm (NSWC/IH drop hammer) <sup>[19]</sup> , 24 (BAM) <sup>[19]</sup>
FS [N]	>360 <sup>[1,2]</sup> , 161.3 <sup>[7,8]</sup> , 800 psi (@ 8 ft/s, 200 µm) <sup>[12]</sup> , insensitive up to 36 kg load <sup>[14]</sup> , >360 <sup>[15]</sup> , p <sub>fr,LL</sub> = 350 MPa <sup>[18]</sup> , p <sub>fr,50%</sub> = 490 MPa <sup>[18]</sup> , no go >353 <sup>[19]</sup> , >353 <sup>[19]</sup>
ESD [J]	0.08 <sup>[1]</sup> , 13.10 <sup>[5]</sup> , 285.5 mJ <sup>[5]</sup> , E <sub>50%</sub> ≥ 8 (200 µm) <sup>[12]</sup> , 250 mJ (est. energy of discharge required to initiate TEX, long-lasting stress generated by electric discharge, current and voltage are oscilloscopically recorded) <sup>[8]</sup> , 6.7 (high voltage pulse with short rise time (µs time range), shock mode) <sup>[8]</sup> , 13.1 (unspecified granulometry) <sup>[19]</sup>
N [%]	21.37
Ω(CO <sub>2</sub> ) [%]	-42.7

$T_{\text{phase transition}}$ [°C]	No indication of phase transition prior to dec. of TEX (DSC @ 10 K/min) <sup>[19]</sup> , ~ 240 (sublimation, TGA) <sup>[19]</sup>
$T_{\text{dec.}}$ [°C]	296.3 (DSC @ 5 °C/min) <sup>[2]</sup> , 262.1 <sup>[14]</sup> , 525 K (DTA onset) <sup>[13]</sup> , 282 (onset, DSC) <sup>[15,19]</sup> , 292.52 (DSC @ 2.5 °C/min) <sup>[17]</sup> , 300.28 (DSC @ 5 °C/min) <sup>[17]</sup> , 302.97 (DSC @ 10 °C/min) <sup>[17]</sup> , 303.46 (DSC @ 20 °C/min) <sup>[17]</sup> , 304 (onset, exo), 311 (exo peak max/DSC @ 10 K/min) <sup>[19]</sup>
$\rho$ [g cm <sup>-3</sup> ]	2.008 <sup>[1]</sup> , 2.19 ± 0.1 (@ 293.15 K) <sup>[3]</sup> , 1.99 <sup>[11,12,14]</sup> , 1.985 (crystal ambient conditions) <sup>[19]</sup> , 2.0076 (X-ray @ 200 K) <sup>[9]</sup> , 2.03 (X-ray @ 100 K) <sup>[20]</sup>
Heat of formation	-541 kJ/mol (enthalpy of form.) <sup>[1]</sup> , -2,064 kJ/kg (enthalpy of form.) <sup>[1]</sup> , -540.9 kJ/mol ( $\Delta_f H$ ) <sup>[11,15]</sup> , -106.5 kcal/mol ( $\Delta_f H$ , exptl.) <sup>[12]</sup> , -541 kJ/mol ( $\Delta_f H$ ) <sup>[19]</sup> , -3,445 kJ/mol ( $\Delta_f H$ , exptl.) <sup>[19]</sup> , -448 kJ/mol ( $\Delta_f H$ , calcd., B3LYP 6-31 + G**) <sup>[19]</sup>
Heat of combustion	2,772 kJ/mol ( $\Delta H_{\text{comb}}$ ) <sup>[19]</sup>

	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{\text{ex}} U^\circ$ [kJ kg <sup>-1</sup> ]	3809	-8.162 (total energy of det., @ 1.985 g cm <sup>-3</sup> , calcd., CHEETAH 2.0) <sup>[15]</sup> $\Delta H_{\text{ex}} = 1,777 \text{ kJ/mol}$ <sup>[19]</sup> $\Delta_{\text{det}} H = -4,481.1 \text{ J/g}$ (calcd., K-J) <sup>[19]</sup>	
$T_{\text{ex}}$ [K]	2729	3,226 (@ 1.985 g cm <sup>-3</sup> , calcd., CHEETAH 2.0) <sup>[15]</sup> 2,631 (@ 1.99 g cm <sup>-3</sup> , $\Delta H_f = -445.6 \text{ kJ/mol}$ , calcd., JAGUAR) <sup>[16]</sup> 1,706 (@ 1.985, TMD, calcd., BKW) <sup>[19]</sup> 3,226 (@ 1.985, TMD, calcd., CHEETAH 1.36) <sup>[19]</sup> 3,190 (@ 1.985, TMD, calcd., CHEETAH 2.0) <sup>[19]</sup> 2,972 (@ 1.985, TMD, calcd., EXPLO 5.0) <sup>[19]</sup>	
$p_{\text{C-J}}$ [GPa]	296	370 katm (@ 1.99 g cm <sup>-3</sup> , calcd. TIGER, BKW) <sup>[12]</sup> 29.2 GPa (@ 1.870 g cm <sup>-3</sup> , calcd. TIGER, BKWR coefficients, BKW equation of state) <sup>[8]</sup> 31 GPa <sup>[14]</sup>	292 <sup>[2]</sup> 294 <sup>[1]</sup>

		<p>31.35 GPa (@ 1.985 g cm<sup>-3</sup>, calcd., CHEETAH 2.0)<sup>[15]</sup></p> <p>32.7 (@ 1.99 g cm<sup>-3</sup>, ΔH<sub>f</sub> = -445.6 kJ/mol, calcd., JAGUAR)<sup>[16]</sup></p> <p>36.5 GPa (@ 1.985, TMD, calcd., BKW)<sup>[19]</sup></p> <p>31.4 GPa (@ 1.985, TMD, calcd., CHEETAH 1.36)<sup>[19]</sup></p> <p>32.24 GPa (@ 1.985, TMD, calcd., CHEETAH 2.0)<sup>[19]</sup></p> <p>29.92 GPa (@ 1.985, TMD, calcd., EXPLO 5.0)<sup>[19]</sup></p> <p>37.0 GPa (@ 1.985, TMD, calcd., TIGER)<sup>[19]</sup></p> <p>31.4 GPa (@ 1.985, TMD, calcd., K-J)<sup>[19]</sup></p>	<p>22.2 GPa (est. based on cylinder test results)<sup>[8]</sup></p> <p>See additional values at the end of section</p>
VoD [m s <sup>-1</sup> ]	8,182 (@ 1.99 g cm <sup>-3</sup> )	<p>8,665 (@ 1.99 g cm<sup>-3</sup>, calcd. TIGER, BKW)<sup>[12]</sup></p> <p>7,689 (@ 1.8 g cm<sup>-3</sup>, calcd. TIGER, BKWR coefficients, BKW equation of state)<sup>[8]</sup></p> <p>7,804 (@ 1.835 g cm<sup>-3</sup>, calcd. TIGER, BKWR coefficients, BKW equation of state)<sup>[8]</sup></p> <p>7,894 (@ 1.870 g cm<sup>-3</sup>, calcd. TIGER, BKWR coefficients, BKW equation of state)<sup>[8]</sup></p> <p>8,164 (@ 1.985 g cm<sup>-3</sup>, calcd., CHEETAH 2.0)<sup>[15]</sup></p> <p>8,510 (@ 1.99 g cm<sup>-3</sup>, ΔH<sub>f</sub> = -445.6 kJ/mol, calcd., JAGUAR)<sup>[16]</sup></p> <p>8,749 (@ 1.985, TMD, calcd., BKW)<sup>[19]</sup></p> <p>8,160 (@ 1.985, TMD, calcd., CHEETAH 1.36)<sup>[19]</sup></p> <p>8,540 (@ 1.985, TMD, calcd., CHEETAH 2.0)<sup>[19]</sup></p> <p>8,683 (@ 1.985, TMD, calcd., CHEETAH 3.0)<sup>[19]</sup></p> <p>8,314 (@ 1.985, TMD, calcd., EXPLO 5.0)<sup>[19]</sup></p> <p>8,665 (@ 1.985, TMD, calcd., TIGER)<sup>[19]</sup></p> <p>8,170 (@ 1.985, TMD, calcd., K-J)<sup>[19]</sup></p>	<p>8,180 (@ 1.9 g cm<sup>-3</sup>)<sup>[11]</sup></p> <p>7,446 (@ 1.815 g cm<sup>-3</sup>)<sup>[2]</sup></p> <p>7,075 (@ 1.87 g cm<sup>-3</sup>, 3% phlegmatized TEX, cylinder test, Cu tube, 25 mm internal diameter, 2.5 mm wall thickness)<sup>[8]</sup></p> <p>8,160 (@ 1.985 g cm<sup>-3</sup>)<sup>[15]</sup></p> <p>TEX belongs to “group 1 explosives” which show an increase in VoD as ρ approaches TMD<sup>[19]</sup></p> <p>See additional data at the end of section</p>

$V_0$ [L kg <sup>-1</sup> ]	631	58.99 mol × 10 <sup>3</sup> of gas per cm <sup>3</sup> TEX wt.% @ 1.985 g cm <sup>-3</sup> , calcd., CHEETAH 2.0 <sup>[15]</sup>	
$I_{sp}$	210 (calcd.) <sup>[19]</sup>		

TEX/wax formulations detonation measurements; a = calcd. with CHEETAH 2.0, b = calcd. TIGER and BKWR set of coefficients, c = confined in Cu tube with 2.5 mm wall thickness<sup>[19]</sup>:

Charge diameter (mm)	Charge $\rho$ (g/cm <sup>3</sup> )	TMD (%)	$V_d$ (exp.) (m/s)	$V_d$ (calcd.) (m/s) <sup>a</sup>	$p_{CJ}$ (exp.) (GPa)	$p_{CJ}$ (calcd.) (GPa)	Gurney velocity (m/s)	Wax % composition
21	1.836	95.2	6,028	—	—	—	—	97% TEX/3% Svit 3RV®
30	1.825	94.7	6,948	—	—	—	—	—
40	1.835	95.2	7,298	—	—	—	—	—
50	1.825	94.7	7,402	—	—	—	—	—
60	1.815	94.1	7,446	—	—	—	—	—
95	1.802	93.5	7,441	7,444 <sup>a</sup>	—	24.35 <sup>a</sup>	—	—
25 <sup>c</sup>	1.87	97.5	7,075	7,988 <sup>a</sup> 7,894 <sup>b</sup>	29.2	26.61 <sup>a</sup> 29.9 <sup>b</sup>	2510	96.5% TEX/3.5 wt. Isobblend®

pressed TEX with 3% wax (\* VoD decreased from 8,500 m/s for first sensors – 5,200 for further sensors. Detonation process probably failed because remains of unreacted TEX were found)<sup>[8]</sup>:

Diameter of charge (mm)	No. of sensors	Distance between sensors (mm)	Total distance between sensors (mm)	Total time (ms)	Average $\rho$ of measured tablets (g cm <sup>-3</sup> )	Average detonation VoD (m/s) <sup>[8]</sup>
21	4	~21	85.9	14.25	1.836	6,028*
30	6	~25	200.8	28.90	1.825	6,948
40	7	~32	229.9	31.50	1.835	7,298
50	7	~23	165.8	22.40	1.825	7,402
60	7	~20	137.0	18.40	1.815	7,446
95	8	~25	175.6	23.60	1.802	7,441

Critical diameter [cm]	Lower $d_c$ of phlegmatized TEX charge with $\rho_0 = 1.836 \text{ g cm}^{-3}$ is $\sim 21 \text{ mm}^{[8]}$ , 60 mm (unconfined state, TEX/wax, 97/3) <sup>[19]</sup> , a 25 mm diameter charge with a slightly lower TEX content (TEX/wax with TEX < 97%) confined by a copper tube sustains detonation, whereas an unconfined sample of 25 mm diameter fails to propagate the shock <sup>[19]</sup> , very large, $\gg 60 \text{ mm}^{[19]}$																												
LSGT [cm]	<p>50% <math>p &gt; 6.98 \text{ GPa}</math> (NOL-LSGT)<sup>[19]</sup></p> <p>Shock sensitivity according to NOL-LSGT with TEX-based formulations, acceptor charge confined within 36.5 mm diameter steel tube<sup>[19]</sup>:</p> <table border="1"> <thead> <tr> <th>Formulation</th> <th>Input pressure (GPa)</th> <th>Test result</th> <th><math>V_d</math> (m/s)</th> </tr> </thead> <tbody> <tr> <td>14.19 PGN, 8.0 DEGDN, 2.0 Desmodur® N-100, 0.81 modifiers, 27.5 AP (200 <math>\mu\text{m}</math>), 27.5 Al (15 <math>\mu\text{m}</math>), 20.0 TEX (200 <math>\mu\text{m}</math>)</td> <td>9.2</td> <td>Fail</td> <td>5579</td> </tr> <tr> <td>14.19 PGN, 8.0 DEGDN, 2.0 Desmodur® N-100, 0.81 modifiers, 27.5 AP (200 <math>\mu\text{m}</math>), 27.5 Al (15 <math>\mu\text{m}</math>), 20.0 TEX (200 <math>\mu\text{m}</math>)</td> <td>6.98</td> <td>Pass</td> <td>No detonation</td> </tr> <tr> <td>17.03 PGN, 9.6 DEGDN, 2.4 Desmodur® N-100, 0.97 modifiers, 70 TEX (200 <math>\mu\text{m}</math>)</td> <td>21.31</td> <td>fail</td> <td>6811</td> </tr> <tr> <td>17.03 PGN, 9.6 DEGDN, 2.4 Desmodur® N-100, 0.97 modifiers, 70 TEX (200 <math>\mu\text{m}</math>)</td> <td>6.98</td> <td>pass</td> <td>No detonation</td> </tr> <tr> <td>2.838 PGN, 1.6 DEGDN, 0.4 Desmodur® N-100, 9.162 modifiers, 95 TEX (200 <math>\mu\text{m}</math>)</td> <td>21.31</td> <td>Fail</td> <td>6263</td> </tr> <tr> <td>2.838 PGN, 1.6 DEGDN, 0.4 Desmodur® N-100, 9.162 modifiers, 95 TEX (200 <math>\mu\text{m}</math>)</td> <td>6.98</td> <td>Fail</td> <td>5571</td> </tr> </tbody> </table>	Formulation	Input pressure (GPa)	Test result	$V_d$ (m/s)	14.19 PGN, 8.0 DEGDN, 2.0 Desmodur® N-100, 0.81 modifiers, 27.5 AP (200 $\mu\text{m}$ ), 27.5 Al (15 $\mu\text{m}$ ), 20.0 TEX (200 $\mu\text{m}$ )	9.2	Fail	5579	14.19 PGN, 8.0 DEGDN, 2.0 Desmodur® N-100, 0.81 modifiers, 27.5 AP (200 $\mu\text{m}$ ), 27.5 Al (15 $\mu\text{m}$ ), 20.0 TEX (200 $\mu\text{m}$ )	6.98	Pass	No detonation	17.03 PGN, 9.6 DEGDN, 2.4 Desmodur® N-100, 0.97 modifiers, 70 TEX (200 $\mu\text{m}$ )	21.31	fail	6811	17.03 PGN, 9.6 DEGDN, 2.4 Desmodur® N-100, 0.97 modifiers, 70 TEX (200 $\mu\text{m}$ )	6.98	pass	No detonation	2.838 PGN, 1.6 DEGDN, 0.4 Desmodur® N-100, 9.162 modifiers, 95 TEX (200 $\mu\text{m}$ )	21.31	Fail	6263	2.838 PGN, 1.6 DEGDN, 0.4 Desmodur® N-100, 9.162 modifiers, 95 TEX (200 $\mu\text{m}$ )	6.98	Fail	5571
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SSGT [cm]	12.5 mm (TEX/PTFE, 95/5, $\rho = 1.85 \text{ g cm}^{-3}$ , BICT-SSGT) <sup>[15]</sup> , SSWGT (small-scale water gap test) reported for TEX-containing formulations are questioned due to the 21 mm diameter of samples being significantly below the critical diameter for TEX, and confinement provided by Plexiglas is weak. <sup>[19]</sup>																																																																					
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Small-scale autoignition test	SBAT (Thiokol): 199 $^{\circ}\text{C}$ (200 $\mu\text{m}$ ) <sup>[12]</sup> , bulk crystalline, 200 $\mu\text{m}$ = mild (burn) response in SBAT @ 252 $^{\circ}\text{C}$ <sup>[19]</sup>																																																																					
Vacuum stability test [ $\text{cm}^3/\text{h}$ ]	0.00 $\text{cm}^3$ @ 110 $^{\circ}\text{C}/20 \text{ h}$ , $\rho_{\text{TEX}} = 1.99 \text{ g cm}^{-3}$ <sup>[10]</sup> , 0.05 mL $\text{g}^{-1}$ @ 110 $^{\circ}\text{C}$ for 20 h <sup>[11,19]</sup> , 0.05 mL/g @ 100 $^{\circ}\text{C}$ after 48 h <sup>[19]</sup> , 0.44 mL/g @ 100 $^{\circ}\text{C}$ for 20 h (CL-20/TEX/HTPB, 32/48/20) <sup>[19]</sup> , 0.04 mL/g @ 100 $^{\circ}\text{C}$ for 20 h (HMA/TEX/HTPB, 32/48/20) <sup>[19]</sup>																																																																					
Thermal stability	Partial detonation in VCCT @ 191 $^{\circ}\text{C}$ (DLE-PO31) <sup>[19]</sup>																																																																					
Vapor pressure [atm @ $^{\circ}\text{C}$ ]	$9.39 \times 10^{-7} \text{ Pa}$ @ ambient temperature <sup>[19]</sup>																																																																					
Solubility [g/mL]	27 mg/L in water <sup>[19]</sup>																																																																					
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Compatibility	<p>Thermal decomposition values, DSC data @ various heating rates<sup>[17]</sup>:</p> <table border="1"> <thead> <tr> <th rowspan="2">Formulation</th> <th colspan="4"><math>T_p</math> (<math>^{\circ}\text{C}</math>)</th> </tr> <tr> <th>2.5 <math>^{\circ}\text{C}/\text{min}</math></th> <th>5 <math>^{\circ}\text{C}/\text{min}</math></th> <th>10 <math>^{\circ}\text{C}/\text{min}</math></th> <th>20 <math>^{\circ}\text{C}/\text{min}</math></th> </tr> </thead> <tbody> <tr> <td>TEX</td> <td>292.52</td> <td>300.28</td> <td>302.97</td> <td>303.46</td> </tr> <tr> <td>TEX/RDX</td> <td>290.52</td> <td>299.27</td> <td>302.11</td> <td>303.11</td> </tr> <tr> <td>TEX/<math>\phi</math>-Pb</td> <td>290.32</td> <td>296.93</td> <td>301.68</td> <td>301.89</td> </tr> <tr> <td>TEX/NC</td> <td>291.28</td> <td>297.94</td> <td>301.78</td> <td>301.97</td> </tr> <tr> <td>TEX/(NC + NG)</td> <td>294.08</td> <td>299.86</td> <td>301.99</td> <td>302.36</td> </tr> <tr> <td>TEX/DINA</td> <td>290.51</td> <td>296.86</td> <td>302.17</td> <td>302.90</td> </tr> <tr> <td>TEX/DEP</td> <td>289.57</td> <td>300.10</td> <td>302.22</td> <td>302.43</td> </tr> <tr> <td>TEX/Al</td> <td>290.68</td> <td>297.90</td> <td>301.59</td> <td>301.99</td> </tr> </tbody> </table> <p><math>\Delta T_p</math> (<math>^{\circ}\text{C}</math>) values @ 10 <math>^{\circ}\text{C}</math> heating rate (DSC)<sup>[17]</sup>:</p> <table border="1"> <thead> <tr> <th>Formulation</th> <th><math>\Delta T_p</math> (<math>^{\circ}\text{C}</math>)</th> <th>Formulation</th> <th><math>\Delta T_p</math> (<math>^{\circ}\text{C}</math>)</th> </tr> </thead> <tbody> <tr> <td>TEX/RDX</td> <td>0.86</td> <td>TEX/DINA</td> <td>0.80</td> </tr> <tr> <td>TEX/<math>\phi</math>-Pb</td> <td>1.29</td> <td>TEX/DEP</td> <td>0.75</td> </tr> <tr> <td>TEX/NC</td> <td>1.19</td> <td>TEX/Al</td> <td>1.38</td> </tr> <tr> <td>TEX/(NC + NG)</td> <td>0.98</td> <td></td> <td></td> </tr> </tbody> </table>	Formulation	$T_p$ ( $^{\circ}\text{C}$ )				2.5 $^{\circ}\text{C}/\text{min}$	5 $^{\circ}\text{C}/\text{min}$	10 $^{\circ}\text{C}/\text{min}$	20 $^{\circ}\text{C}/\text{min}$	TEX	292.52	300.28	302.97	303.46	TEX/RDX	290.52	299.27	302.11	303.11	TEX/ $\phi$ -Pb	290.32	296.93	301.68	301.89	TEX/NC	291.28	297.94	301.78	301.97	TEX/(NC + NG)	294.08	299.86	301.99	302.36	TEX/DINA	290.51	296.86	302.17	302.90	TEX/DEP	289.57	300.10	302.22	302.43	TEX/Al	290.68	297.90	301.59	301.99	Formulation	$\Delta T_p$ ( $^{\circ}\text{C}$ )	Formulation	$\Delta T_p$ ( $^{\circ}\text{C}$ )	TEX/RDX	0.86	TEX/DINA	0.80	TEX/ $\phi$ -Pb	1.29	TEX/DEP	0.75	TEX/NC	1.19	TEX/Al	1.38	TEX/(NC + NG)	0.98		
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	Compatible with a large number of inert and energetic binders, for example, PGN/DEGN/Desmodur® N-100 <sup>[19]</sup> , compatible with DETN, EDDN, NTO, GUDN, RDX, HMX, NC, NQ, NG and GAP (DSC, onset for selected energetic materials and their 1:1 mixtures with TEX) <sup>[19]</sup> :				
Material	Exotherm onset (°C)	Peak (°C)	ΔT onset (°C)	ΔT peak (°C)	
TEX	304	308			
NTO	274	277			
NQ	250	255			
GUDN	222	226			
RDX	219	248			
NC	203	214			
NG	187	204			
NTO/TEX	260	267	-14	-10	
NQ/TEX	245	251	-5	-4	
GUDN/TEX	220	223	-2	-3	
RDX/TEX	222	250	+3	+2	
NC/TEX	203	214	0	0	
NG/TEX	181	201	-6	-3	

	TEX <sup>[9,19]</sup>	TEX <sup>[19,20]</sup>
Chemical formula	C <sub>6</sub> H <sub>6</sub> N <sub>4</sub> O <sub>8</sub>	C <sub>6</sub> H <sub>6</sub> N <sub>4</sub> O <sub>8</sub>
Molecular weight [g mol <sup>-1</sup> ]	262.15	262.15
Crystal system	Triclinic	Triclinic
Space group	P-1 (no. 2)	P-1 (no. 2)
<i>a</i> [Å]	6.8360(12)	6.814(1)
<i>b</i> [Å]	7.6404(14)	7.622(1)
<i>c</i> [Å]	8.7765(16)	8.733(1)
α [°]	82.37(2)	82.23(1)
β [°]	75.05(2)	75.02(1)
γ [°]	79.46(2)	79.45(1)
<i>V</i> [Å <sup>3</sup> ]	433.64(14)	428.8(1)
<i>Z</i>	2	2
<i>ρ</i> <sub>calc</sub> [g cm <sup>-3</sup> ]	2.0076(6)	2.03
<i>T</i> [K]	200	100

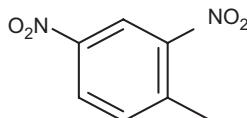
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## 2,4-Dinitrotoluene

Name [German, acronym]: 1-Methyl-2,4-dinitrobenzene,  
2,4-dinitrotoluene [2,4-DNT]

Main (potential) use: TNT precursor, ingredient in plastic explosives,  
dynamites, ingredient in smokeless powders<sup>[19]</sup>,  
gelatinizer for propellant powders<sup>[19]</sup>, ingredient of  
propellant powders, dynamites and plastic explosives<sup>[2]</sup>

Structural formula:



	<b>2,4-DNT</b>
Formula	C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> O <sub>4</sub>
Molecular mass [g mol <sup>-1</sup> ]	182.14
Appearance at RT	Yellow solid <sup>[2,16]</sup> , lemon-yellow crystals <sup>[19]</sup>
IS [J]	>40 (<100 µm), H <sub>50%</sub> = 70 cm (2 kg mass) <sup>[5]</sup> , H <sub>50</sub> ≥ 90 cm (design no. 3 apparatus) <sup>[28]</sup> , H <sub>50</sub> = 58 cm (design no. 5 apparatus) <sup>[28]</sup>
FS [N]	>360 (<100 µm), unaffected by steel shoe (friction pendulum test) <sup>[2]</sup> , unaffected by fiber shoe (friction pendulum test) <sup>[2]</sup>
ESD [J]	>1.5 (<100 µm)
N [%]	15.38
Ω(CO <sub>2</sub> ) [%]	-114.20
T <sub>m.p.</sub> [°C]	71 <sup>[2,5,20,26]</sup> , 70.5 <sup>[4]</sup> , 70 <sup>[11,18,19]</sup> , 72 <sup>[15]</sup> , 69.5 <sup>[16]</sup>
T <sub>b.p.</sub> [°C]	300 (dec.) <sup>[2,11,19]</sup> , 300 <sup>[26]</sup>
T <sub>dec</sub> [°C]	300 (dec.) <sup>[2,11,19]</sup> , 586.2 K (DSC) <sup>[27]</sup>
ρ [g cm <sup>-3</sup> ]	1.559 (@ 173 K), 1.513 (@ 298 K), 1.521 <sup>[2,4,5,15]</sup> , sp. gr. = 1.32 (@ 15 °C) <sup>[19]</sup> , 1.32 <sup>[14]</sup> , 1.52 <sup>[17]</sup> , 1.52 (crystal) <sup>[18]</sup>
Heat of formation	-292.8 kJ/kg (energy of form.) <sup>[4]</sup> , -374.7 kJ/kg (enthalpy of form.) <sup>[4]</sup> , 54.9 kcal/kg <sup>[21]</sup> , 31.3 kcal/mol (Q <sub>f</sub> ) <sup>[5]</sup> , -52.7 kJ/mol (Δ <sub>f</sub> H <sup>o</sup> ) <sup>[14]</sup>
Heat of combustion	853.7 kcl/mol (Q <sub>c</sub> <sup>V</sup> ) <sup>[5]</sup> , 1,545 cal/g <sup>[2]</sup> , 4,660 kcal/kg (@ C <sup>V</sup> ) <sup>[21]</sup>

	Calcd. (EXPLO5 6.03)	Exptl.
$-\Delta_{\text{ex}}U^\circ [\text{kJ kg}^{-1}]$	3,613	3,192 [ $\text{H}_2\text{O(l)}$ ] <sup>[1,4]</sup> 3,050 [ $\text{H}_2\text{O(g)}$ ] <sup>[4]</sup> 1,056 kcal/kg <sup>[5]</sup>
$T_{\text{ex}} [\text{K}]$	2,707	
$p_{\text{CJ}} [\text{kbar}]$	158	
$\text{VoD} [\text{m s}^{-1}]$	6,098 (@ TMD)	3,850 (@ 1.0 g/cc, steel tubes of 28–30 mm diameter) <sup>[5]</sup> 5,900 (@ 1.52 g/cc, 60 mm tube) <sup>[5]</sup> (see table below)
$V_0 [\text{L kg}^{-1}]$	615	807 <sup>[3,4]</sup> 602 <sup>[5]</sup>

Detonation velocity measurements on fine DNT<sup>[18]</sup>:

$p_0 (\text{g/cc})$	$d (\text{cm})$	$D (\text{mm}/\mu\text{s})$		$D1$	$D2$	
1.302	3.81	4.722		4.704	4.708	
1.301	5.08	5.120		5.075	5.081	$D_i (1.301 \text{ g/cc}) = 5.63 \text{ mm}/\mu\text{s}$
1.301	7.62	5.333		5.252	5.266	
				$D (1.507)$		
1.5061	2.54	5.395		5.386	5.387	
1.5071	3.495	5.700		5.681	5.684	
1.5111	5.08	5.864	5.850	5.798	5.802	$D_i (1.507 \text{ g/cc}) = 6.23 \text{ mm}/\mu\text{s}$
1.4951	7.62	6.032	6.075	5.983	5.993	
1.001	5.008	$F$		$F$		
1.157		3.751		3.718	3.726	
1.226		4.685		4.653	4.660	
1.408		5.512		5.464	5.468	
1.511		5.864		5.812	5.816	
1.001	7.62	3.590		3.520	3.542	

*D* measurements by probes on coarse DNT, charges confined in 12 in length of standard gap test tubing bored to take probes<sup>[18]</sup>:

Shot no.	$\rho_0$ (g/cc)	<i>D</i> (mm/ $\mu$ s)	$\Sigma$
1	1.00	3.788	0.013
2	1.00	3.772	0.037
3	1.50	Failed	
4	1.50	5.908	0.051

Failures observed on fine DNT<sup>[18]</sup>:

<i>d</i> (cm)	$\rho_0$ (g/cc)	Failure at (cm)
5.08	1.001	15.2
2.54	0.800*	5.7
↓	1.001*	15.2
	1.204	6.6 <sup>†</sup>
	1.406	9.9
	1.5141 <sup>§</sup>	<10.2 <sup>‡</sup>
	1.5071 <sup>§</sup>	<7.9 <sup>‡</sup>

\*Preliminary lab sample of 10–15  $\mu$ m DNT; <sup>†</sup>booster only 2.54 cm long; <sup>‡</sup>unreacted DNT recovered

Summary of detonability data from ref.<sup>[18]</sup>:

$\rho_0$ (g/cc)	<i>d</i> <sub>+</sub> (cm)	<i>d</i> <sub>–</sub> (cm)
1.00	7.62	5.08
1.16	5.08*	2.54
1.30	3.81*	2.54
1.40	5.08	2.54
1.506	2.54	–
1.514	–	2.54

\*Record suggests this is very near *d*<sub>c</sub>.

Critical diameter [cm]	Fine DNT (10 $\mu$ m) <sup>[18]</sup> :						
	Critical diameter for detonation, <i>d</i> <sub>c</sub> (mm)						
	70	75	80	85	90	93	98
	58	51.5	44.5	38	31.5	28	25

Trauzl test [cm <sup>3</sup> , % TNT]	64% TNT <sup>[2,6]</sup> , 240 cm <sup>3</sup> (10 g sample) <sup>[4]</sup> , 240 <sup>[24]</sup>				
Sand test [g]	19.3 g sand crushed (200 g sand test) <sup>[2,5]</sup>				
Ballistic mortar test	71% TNT <sup>[2,6]</sup>				
Initiation efficiency	0.20 g LA minimum detonating charge <sup>[2]</sup> , 0.25 g tetryl minimum detonating charge <sup>[2]</sup>				
Gap test	Shock sensitivity tests on coarse DNT <sup>[18]</sup> :				
	$\rho_0$ (g/cc)	% TMD	Gap test extended/regular (no. cards)	$P_g$ (kbar)	Comments
	0.704	46.3	~ 190	—	In view of $D(\rho_0, d)$ pattern material probably not detonating
	0.999	65.9	181	21.5	Probably near fail limit
	1.5021	98.9		105	Near-dead press limit
	1.453	Cast	12*		Definitely not detonating
*Result negative with double length tube.					
Regular gap test, coarser DNT than in table earlier <sup>[18]</sup> :					
	$\rho_0$ (g/cc)	% TMD	No. cards	$p_g$ (kbar)	Comments
	1.100	72.3	143	33.3	Reversal of trend and since this charge is coarser suggests this charge was not detonating
	1.203	79.1	144	32.5	
	1.271	83.7	137	35.4	
	1.397	91.8	115	43.7	
	1.4921	98.1	85	55.9	
	Zero gap, regular test				
	1.5071	99.1	Positive		Double length tube
	1.5151	99.7	Positive		This material cannot be dead pressed in dimensions of regular gap test
	1.5181	99.9	Positive		
	Zero gap, regular test with acceptor scaled to 0.70				
	1.3151	86.5	Positive		
	1.3571	89.3	Positive		
	1.4071	92.6	Positive		
	1.4701	92.7	Negative		Material does dead press @ 0.7 scale of regular test

LSGT [cm]	50% gap, all charges isostatically pressed (whether the values are for 2,4-DNT or 2,6-DNT was not specified) <sup>[21]</sup> :																																																																				
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Vacuum stability test [cm <sup>3</sup> /h]	0.04 <sup>[5]</sup> , 0.04 cc/40 h @ 120 °C <sup>[2]</sup>																																																																				
Steel sleeve	Thermal ignition by steel sleeve: limiting diameter = 1 mm, time to ignition = 49 s, combustion time = 21 s <sup>[5]</sup>																																																																				

Vapor pressure [atm @ °C]	$2.2 \times 10^{-4}$ Torr @ 25 °C <sup>[11]</sup> , $2.17 \times 10^{-4}$ Torr @ 25 °C <sup>[15]</sup> , $1.47 \times 10^{-4}$ mm Hg @ 25 °C <sup>[20]</sup>																																										
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Solubility [g/mL]	270 mg/L in H <sub>2</sub> O @ 22 °C <sup>[11]</sup> , aqueous solubility = 280 mg/L @ 25 °C <sup>[15]</sup> , 0.28 g/L in H <sub>2</sub> O @ 25 °C <sup>[17]</sup> , 270 mg/L in H <sub>2</sub> O @ 25 °C <sup>[20]</sup>																																										
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Hygroscopicity	0.00% @ 25 °C in 100% RH <sup>[2]</sup>			
Photosensitivity	Effect of UV continuous-flow treatment on aqueous 2,4-DNT solutions <sup>[12]</sup> :			
	UV exposure (h)	LC 2,4-DNT (ppm)	pH	TLC detectable products
	0	65.3	6.7	2,4-DNT
	2	0.4	3.9	1 <sup>f</sup>
	4	0.2	3.6	1 <sup>f</sup>
	6	0	3.5	1 <sup>f</sup>
	8	0	3.5	1 <sup>f</sup>
	1 <sup>f</sup> = one unidentified product was detected which fluoresces at 375 nm.			
	UV – 0.1% H <sub>2</sub> O <sub>2</sub> static system treatment of aqueous 2,4-DNT solutions (100 ppm 2,4-DNT) <sup>[12]</sup> :			
	UV exposure time (h)	ppm H <sub>2</sub> O <sub>2</sub>	TOC analyzer	
	0	1,000	38.4	
	1	> 12, < 50	2.4	
	2	~ 1	–	
	5	0	–	
	Sunlight photolysis of 1.0 ppm 2,4-DNT in water gave half-lives of 43 h (distilled water) <sup>[25]</sup> , 2.7 h (river water) <sup>[25]</sup> , 9.6 h (bay water) <sup>[25]</sup> , 3.7 h (pond water) <sup>[25]</sup>			
ΔH <sub>sub</sub> [kJ/mol]	99.6 (exptl.) <sup>[13]</sup> , 90.6 (calcd., QSPR) <sup>[13]</sup>			
Diffusion coefficient [cm <sup>2</sup> /s]	0.067 (air) <sup>[15]</sup> , 7.31 × 10 <sup>-6</sup> (water) <sup>[15]</sup>			
Heat of fusion [cal/g]	109 kJ/kg <sup>[4]</sup> , 26.1 <sup>[15]</sup>			
Heat of decomposition [kJ/mol]	850 (Q <sub>dec</sub> , DSC) <sup>[27]</sup>			
Log K <sub>ow</sub>	1.98 <sup>[15,17,20]</sup>			
Log K <sub>oc</sub>	2.40 <sup>[15]</sup> , 282 (K <sub>oc</sub> ) <sup>[25]</sup>			

Lead cylinder test	Lead cylinder test of DNT ( <sup>a</sup> charges initiated with No. 8 cap, no booster used, charge length = 100 mm. When a 10 g tetryl booster was used against an inert (hexamethylenetetramine at unspecified density), the control was 9 mm; <sup>b</sup> at this density, $d_c$ of unconfined charge was reported as 45 mm. On comparable material at 0.7 g/cc $d_c > 76$ mm was found; <sup>c</sup> detonation may have occurred), Blinov's values from ref. <sup>[18]</sup>					
	Casing	Casing diameter (mm)	Casing wt/length (g/cm)	Decrease in height of lead cylinder <sup>a</sup> , $\Delta h$ , mm	$\Delta h/\rho_0$	
		Inner	Outer			
	$\rho_0 = 0.6 \text{ g/cc}^b$					
	Steel with seam	40	48	38	16.1	26.8
	Steel with seam and slit	40	48	38	12.8	21.3
	Lead	40	44	30	21.3	35.4 <sup>c</sup>
	H <sub>2</sub> O	40	80	40	13.7, 15.0	22.8, 25.0
	Clay	40	64	40	17.0, 14.6	28.3, 24.3
	Tin	40	41.2	3	15.2, 15.6	25.3, 26.0
	$\rho_0 = 0.8 \text{ g/cc}$					
	Steel with seam	40	48	40	26.4	33.0 <sup>c</sup>
	Steel with seam and slit	40	48	40	25.0	31.2 <sup>c</sup>
	Lead	40	46	40	26.0	32.5 <sup>c</sup>
	H <sub>2</sub> O	40	80	40	1.2, 1.2	1.5, 1.5
	Clay	40	64	40	1.5	1.9
	Tin	40	41.2	7	1.0, 0.8	1.3, 1.0
Rifle bullet impact test	100% unaffected in trials <sup>[2]</sup>					
65.5 °C KI test	60 + min <sup>[2]</sup>					
Thermal conductivity [cal/s/cm/°C]	$6.28 \times 10^{-4}$ @ 1.322 g cm <sup>-3</sup> <sup>[2]</sup>					
Dipole moment [D]	4.33 (benzene soln. @ 25 °C) <sup>[29]</sup> , 4.90 (calcd., gas @ 25 °C, MINDO/3) <sup>[29]</sup>					

	2,4-Dinitrotoluene <sup>[8]</sup>	2,4-Dinitrotoluene <sup>[9]</sup>	2,4-Dinitrotoluene <sup>[10]</sup>
Chemical formula	C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> O <sub>4</sub>	C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> O <sub>4</sub>	C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> O <sub>4</sub>
Molecular weight [g mol <sup>-1</sup> ]	182.14	182.14	182.14
Crystal system		Monoclinic	Monoclinic
Space group		P2 <sub>1</sub> /n (no.14)	P2 <sub>1</sub> /n (no.14)
a [Å]	12.86	8.126(2)	8.0057(7)
b [Å]	15.27	15.217(4)	15.1273(18)
c [Å]	8.15	12.998(2)	12.8853(13)
α [°]	90	90	90
β [°]	95.15	94.77(2)	95.877(6)
γ [°]	90	90	90
V [Å <sup>3</sup> ]	1,593.97	1,601.68	1,552.3(3)
Z	8	8	8
ρ <sub>calc</sub> [g cm <sup>-3</sup> ]	1.518	1.511	1.559
T [K]	295	298	173

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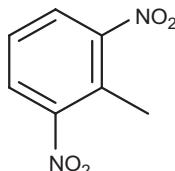
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## 2,6-Dinitrotoluene

Name [German, acronym]: 2-Methyl-1,3-dinitrobenzene, 2,6-dinitrotoluene  
[2,6-DNT]

Main (potential) use: TNT precursor

Structural formula:



	<b>2,6-DNT</b>
Formula	C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> O <sub>4</sub>
Molecular mass [g mol <sup>-1</sup> ]	182.14
Appearance at RT	
IS [J]	>40 (<100 µm), H <sub>50%</sub> = 66 cm <sup>[4]</sup> , 50 Nm no reaction <sup>[3]</sup>
FS [N]	>360 (<100 µm), no reaction ≤ 353 N <sup>[3]</sup>
ESD [J]	>1.5 (<100 µm)
N [%]	15.38
Ω(CO <sub>2</sub> ) [%]	-114.20
T <sub>m.p.</sub> [°C]	56, 64–66 <sup>[7,11]</sup> , 66 <sup>[10,16]</sup> , 71 <sup>[2]</sup>
T <sub>b.p.</sub> [°C]	285 <sup>[16]</sup>
T <sub>dec</sub> [°C]	630.0 K (DSC) <sup>[18]</sup>
ρ [g cm <sup>-3</sup> ]	1.548 (@ 293 K), 1.538 <sup>[3,10]</sup> , 1.515 (gas pycnometer), 1.538 (@ RT) <sup>[4]</sup> , 1.2833 (@ 111 °C) <sup>[4]</sup> , 1.521 <sup>[2]</sup> ,
Heat of formation	-159.5 kJ/kg (energy of form.) <sup>[3]</sup> , -241.2 kJ/kg (enthalpy of form.) <sup>[3]</sup> , 34.8 kcal/kg <sup>[2]</sup> , 29.6 kcal/mol (Q <sub>f</sub> ) <sup>[4]</sup> , 13.6 kcal/mol (Δ <sub>f</sub> H (g) <sup>o</sup> , calcd., ccCA-P) <sup>[17]</sup> , 9.3 kcal/mol (Δ <sub>f</sub> H (g) <sup>o</sup> , calcd., ccCA-S3) <sup>[17]</sup> , 11.5 kcal/mol (Δ <sub>f</sub> H (g) <sup>o</sup> , calcd., ccCA-PS3) <sup>[17]</sup> , 7.9 kcal/mol (Δ <sub>f</sub> H (g) <sup>o</sup> , calcd., G3) <sup>[17]</sup> , 10.3 kcal/mol (Δ <sub>f</sub> H (g) <sup>o</sup> , calcd., G3(MP2)) <sup>[17]</sup> , -9.6 kcal/mol (Δ <sub>f</sub> H (g) <sup>o</sup> , exptl.) <sup>[17]</sup>
Heat of combustion	855.2 kcal/mol (Q <sub>c</sub> ) <sup>[4]</sup> , 4,691 kcal/kg (@ Q <sub>cV</sub> ) <sup>[12]</sup>
	Calcd. (EXPLO5 6.03) Exptl.

$-\Delta_{\text{ex}} U^{\circ} [\text{kJ kg}^{-1}]$	3,697	1,085 kcal/kg ( $Q_e$ ) <sup>[4]</sup> 3,325 [ $\text{H}_2\text{O (l)}$ ] <sup>[1,3]</sup> 3,183 [ $\text{H}_2\text{O (g)}$ ] <sup>[3]</sup>
$T_{\text{ex}} [\text{K}]$	2,747	
$p_{\text{CJ}} [\text{kbar}]$	159	
VoD [ $\text{m s}^{-1}$ ]	6,125 (@ TMD)	
$V_0 [\text{L kg}^{-1}]$	1,716	807 <sup>[2,3]</sup>

Critical diameter [cm]	1 mm (steel sleeve test) <sup>[3]</sup>					
Trauzl test [ $\text{cm}^3$ , % TNT]	240 $\text{cm}^3$ (10 g sample) <sup>[3]</sup> , 260 $\text{cm}^3$ <sup>[15]</sup>					
LSGT [cm]	50% gap, all charges isostatically pressed (whether the values are for 2,4-DNT or 2,6-DNT was not specified) <sup>[13]</sup> :					
	TMD ( $\text{g cm}^{-3}$ )	Exptl. $\rho$ ( $\text{g cm}^{-3}$ )	% TMD	gap (cards)		
	1.521 (350 $\mu\text{m}$ )	1.49	98.1	85		
	1.521 (150 $\mu\text{m}$ )	1.50	98.9	24		
	Data for DNT – isomer not specified (c = cast, P = packed by hand, I = isostatic press, H = hydraulic press; tests all regular type unless listed as extended E, all charges are conditioned and fired @ 25 °C unless stated otherwise) <sup>[14]</sup> :					
	Density		50% point		Particle size ( $\mu\text{m}$ )	comments
g/cc	% TMD	Cards	kbar			
0.71P	46.5	192 ± 2 E	22	150		
1.00 H	65.7	181 E	25	150	Go at 0 gap DLT extended (DLT = double length tube)	
1.50I	98.9	24	103	150		
1.45 C	95.5	12 E	128	150	2 DLT extended tests failed at 0 gap	
1.10H	72.3	143 ± 1	40	350	Probably not detonating	
1.20 H	79.1	144	39	350		
1.27 H	83.6	137	43	350		
1.40 H	91.8	115	50	350	23 °C	
1.49I	98.1	85 ± 2	61	350	23 °C	

5 s explosion $T$ [°C] Deflagration $T$ [°C]	360 <sup>[5]</sup> , 360 (ignition) <sup>[3]</sup>																																							
Vapor pressure [atm @ °C]	$5.67 \times 10^{-4}$ Torr @ 20 °C <sup>[7,10]</sup> , $5.7 \times 10^{-4}$ mm Hg @ 25 °C <sup>[11]</sup> , $3.5 \times 10^{-4}$ mm Hg @ 20 °C <sup>[16]</sup>																																							
Solubility [g/mL]	206 mg/L H <sub>2</sub> O @ 25 °C <sup>[7,10,11]</sup>																																							
Photosensitivity	<p>Effect of UV continuous-flow treatment on aqueous 2,6-DNT solutions<sup>[8]</sup>:</p> <table border="1"> <thead> <tr> <th>UV exposure (h)</th> <th>LC 2,6-DNT (ppm)</th> <th>pH</th> <th>TLC detectable products</th> </tr> </thead> <tbody> <tr> <td>0</td> <td>91</td> <td>6.3</td> <td>2,6-DNT</td> </tr> <tr> <td>2</td> <td>1.7</td> <td>3.5</td> <td>0</td> </tr> <tr> <td>4</td> <td>0</td> <td>3.7</td> <td>0</td> </tr> <tr> <td>6</td> <td>0</td> <td>3.7</td> <td>0</td> </tr> <tr> <td>8</td> <td>0</td> <td>3.8</td> <td>0</td> </tr> </tbody> </table> <p>UV – 0.1% H<sub>2</sub>O<sub>2</sub> static treatment of aqueous 2,6-DNT solns. (100 ppm 2,6-DNT)<sup>[8]</sup>:</p> <table border="1"> <thead> <tr> <th>UV exposure time (h)</th> <th>ppm H<sub>2</sub>O<sub>2</sub></th> <th>TOC analyzer</th> </tr> </thead> <tbody> <tr> <td>0</td> <td>1000</td> <td>45.3</td> </tr> <tr> <td>1</td> <td>&gt; 12, &lt; 50</td> <td>3.15</td> </tr> <tr> <td>2</td> <td>1</td> <td>–</td> </tr> <tr> <td>5</td> <td>0</td> <td>–</td> </tr> </tbody> </table>	UV exposure (h)	LC 2,6-DNT (ppm)	pH	TLC detectable products	0	91	6.3	2,6-DNT	2	1.7	3.5	0	4	0	3.7	0	6	0	3.7	0	8	0	3.8	0	UV exposure time (h)	ppm H <sub>2</sub> O <sub>2</sub>	TOC analyzer	0	1000	45.3	1	> 12, < 50	3.15	2	1	–	5	0	–
UV exposure (h)	LC 2,6-DNT (ppm)	pH	TLC detectable products																																					
0	91	6.3	2,6-DNT																																					
2	1.7	3.5	0																																					
4	0	3.7	0																																					
6	0	3.7	0																																					
8	0	3.8	0																																					
UV exposure time (h)	ppm H <sub>2</sub> O <sub>2</sub>	TOC analyzer																																						
0	1000	45.3																																						
1	> 12, < 50	3.15																																						
2	1	–																																						
5	0	–																																						
$\Delta H_{\text{sub}}$ [kJ/mol]	98.3 (exptl.) <sup>[9]</sup> , 90.6 (calcd., QSPR) <sup>[9]</sup>																																							
Heat of fusion [cal/g]	94 kJ/kg <sup>[3]</sup> , 22.5 <sup>[10]</sup>																																							
Diffusion coefficient [cm <sup>2</sup> /s]	0.067 (air) <sup>[10]</sup> , $7.31 \times 10^{-6}$ (water) <sup>[10]</sup>																																							
Log $K_{\text{ow}}$	1.89 <sup>[10]</sup> , 2.02 <sup>[10,11]</sup> , 1.72 <sup>[16]</sup>																																							
Log $K_{\text{oc}}$	1.89 <sup>[10]</sup> , 204 ( $K_{\text{oc}}$ , est.) <sup>[16]</sup>																																							
Heat of decomposition [kJ/mol]	718 ( $Q_{\text{dec.}}$ , DSC) <sup>[18]</sup>																																							
Dipole moment [D]	2.81 (benzene soln. @ 25 °C) <sup>[19]</sup> , 3.51 (calcd., (g) @ 25 °C, MINDO/3) <sup>[19]</sup>																																							

	2,6-Dinitrotoluene <sup>[5]</sup>	2,6-Dinitrotoluene <sup>[6]</sup>
Chemical formula	C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> O <sub>4</sub>	C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> O <sub>4</sub>
Molecular weight [g mol <sup>-1</sup> ]	182.14	182.14
Crystal system	Orthorhombic	Orthorhombic

Space group		<i>P2<sub>1</sub>2<sub>1</sub>2<sub>1</sub></i>
<i>a</i> [Å]	7.82	7.830(2)
<i>b</i> [Å]	13.70	13.683(3)
<i>c</i> [Å]	7.39	7.296(2)
$\alpha$ [°]	90	90
$\beta$ [°]	90	90
$\gamma$ [°]	90	90
<i>V</i> [Å <sup>3</sup> ]	791.72	781.7(3)
<i>Z</i>	4	4
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.528	1.548
<i>T</i> [K]	295	293

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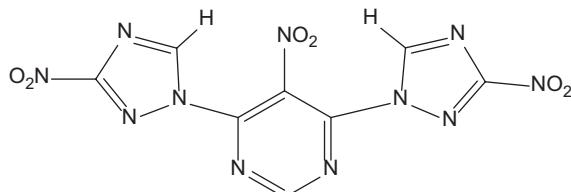
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## 4,6-Di-2(5-nitro-1,2,4-triazole)-5-nitropyrimidine

Name [German, acronym]: 4,6-Di-2(5-nitro-1,2,4-triazole)-5-nitropyrimidine,  
 [4,6-di-2(5-nitro-1,2,4-triazol)-5-nitropyrimidin]

Main (potential) use: Possible use as secondary explosive<sup>[1]</sup>

Structural formula:



	4,6-Di-2(5-nitro-1,2,4-triazole)-5-nitropyrimidine		
Formula	C <sub>8</sub> H <sub>3</sub> N <sub>11</sub> O <sub>6</sub>		
Molecular mass [g mol <sup>-1</sup> ]	349.18		
Appearance at RT	White crystals <sup>[1]</sup>		
IS [J]	>72 cm (5 kg mass, 30 mg sample, sandpaper) <sup>[1]</sup>		
N [%]	44.13		
Ω(CO <sub>2</sub> ) [%]	-55.78		
T <sub>m,p.</sub> [°C]	248 <sup>[1]</sup>		
ρ [g cm <sup>-3</sup> ]	1.74 (gas pycnometry) <sup>[1]</sup>		
Heat of formation			
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
-Δ <sub>ex</sub> U <sup>o</sup> [kJ kg <sup>-1</sup> ]			
T <sub>ex</sub> [K]			
p <sub>C<sub>j</sub></sub> [kbar]			
VoD [m s <sup>-1</sup> ]		8,420 (@ 1.74 g cm <sup>-3</sup> , calcd., R-P method) <sup>[1]</sup>	
V <sub>0</sub> [L kg <sup>-1</sup> ]			
5 s explosion T [°C]	380 (5 s. deflagration T) <sup>[1]</sup>		
Deflagration T [°C]	356 (deflag., @ 5 °C/min) <sup>[1]</sup>		

Solubility [g/mL]	Soluble in acetone, methyl ethyl acetone, ethyl acetate, CH <sub>3</sub> CN, dimethylacetamide, DMF, DMSO and nitrobenzene <sup>[1]</sup> , insoluble in water <sup>[1]</sup> , recryst. from CH <sub>3</sub> CN <sup>[1]</sup>
Specific surface	2.70 m <sup>2</sup> (measured, BET method) <sup>[1]</sup>

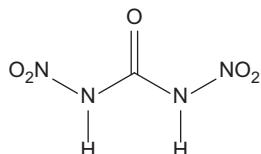
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## Dinitrourea

Name [German, acronym]: *N,N'*-Dinitrourea [dinitroharnstoff, DNU]

Main (potential) use: Precursor in the synthesis of nitramines<sup>[3,4]</sup>, precursor in synthesis of nitramide<sup>[8]</sup>

Structural formula:



	<b>DNU</b>
Formula	$\text{CH}_2\text{N}_4\text{O}_5$
Molecular mass [g mol <sup>-1</sup> ]	150.05
Appearance at RT	White solid <sup>[4]</sup>
IS [J]	5 (50% initiation prob., BAM, 2 kg mass) <sup>[1]</sup> , 5 (BAM) <sup>[4]</sup> , 5 (2 kg mass, 50% prob., BAM) <sup>[7]</sup> , 3 (2 kg mass, $\frac{1}{6}$ positive tests, BAM) <sup>[7]</sup>
FS [N]	76 (50% initiation prob., up-down method) <sup>[1]</sup> , 76 (BAM) <sup>[4]</sup> , 76 (50% prob., BAM) <sup>[7]</sup> , 27 ( $\frac{1}{6}$ positive tests, BAM) <sup>[7]</sup>
N [%]	37.34
$\Omega(\text{CO}_2)$ [%]	+21.33
$T_{\text{m.p.}}$ [°C]	90 <sup>[2]</sup> , 101–104 (with dec., capillary) <sup>[8]</sup> , 107–110 (with dec., Boetius heating plate) <sup>[8]</sup>
$T_{\text{dec.}}$ [°C]	100 (onset), 120 (steep exothermic dec.) (DSC @ 10 °C/min, Al cups with pierced lids) <sup>[1]</sup> , 80–90 (mass loss begins), 110–120 (steep mass loss) (TGA @ 10 °C/min, Al cups) <sup>[1,7]</sup> , ~100 (exo, onset), ~124 (exo, peak max) ~132 (small exo peak max) (DSC @ 10 °C/min, N <sub>2</sub> atmosphere, Al cups with pierced lids) <sup>[7]</sup> , dec. @ RT in the presence of H <sub>2</sub> O and traces of acids – can lead to spontaneous ignition <sup>[3]</sup> , stability strongly depends on its purity <sup>[3]</sup> , stability depends on purity – 80% pure DNU undergoes self-ignition on storing @ 25 °C for 20 min <sup>[4]</sup> , thermal stability of DNU is very sensitive to air humidity <sup>[6]</sup> , >75, accelerated >90 (sample linear heating) <sup>[6]</sup> , 100 (exo peak, DSC) <sup>[6]</sup> , 101–104 (melts with dec., capillary) <sup>[8]</sup> , 107–110 (melts with dec., Boetius heating plate) <sup>[8]</sup> , stable up to 80 °C DSC/TGA @ 10 °C/min, at higher heating rates, sharp mass loss in 110–120 °C range with intense dec. @ 147–149 °C <sup>[8]</sup>
$\rho$ [g cm <sup>-3</sup> ]	1.98 <sup>[1,2,4]</sup> , 1.98 (calc.) <sup>[2]</sup> , 1.98 (He gas pycnometry) <sup>[7]</sup> , 1.98 (flootation method) <sup>[8]</sup> , 2.067 (single-crystal X-ray diffraction @ 90 K) <sup>[8]</sup> , 2.33 (PM3/VSTO-3G calcd.) <sup>[8]</sup>

Heat of formation	24.88 ( $\Delta H^\circ_{298}$ (g), calc., G3MP2 method, isodesmic rxns.) <sup>[2]</sup> , -58.8 ( $\Delta_f H^\circ_{298}$ (s), est.) <sup>[2]</sup> , + 24.88 kJ/mol (heat of formation (g), calc., G3MP2 method based on isodesmic reactions) <sup>[5]</sup> , -230 kJ mol <sup>-1</sup> (formation enthalpy, est.) <sup>[6]</sup>		
	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^\circ$ [kJ kg <sup>-1</sup> ]			
$T_{\text{ex}}$ [K]			
$p_{\text{C-J}}$ [kbar]		36.1 GPa (calcd. CHEETAH 4.0) <sup>[2,4]</sup>	
VoD [m s <sup>-1</sup> ]		8,861 (calcd. CHEETAH 4.0) <sup>[2,4]</sup>	
$V_0$ [L kg <sup>-1</sup> ]			
5 s explosion $T$ [°C] Ignition $T$ [°C]	147–149 <sup>[3]</sup> , crude DNU still containing nitrating acids maintained @ 25 °C for 20 min undergoes self-ignition <sup>[3]</sup> , 91–93 <sup>[4]</sup> , 91–93 (Wood's metal bath) <sup>[2]</sup> , 91–93 (300 s, Wood's metal bath) <sup>[7]</sup> , 101.4 (heating in air with rel. humidity = 74%, 100% mass loss) <sup>[6]</sup> , 103.5 (heating under Ar, 100% mass loss) <sup>[6]</sup> , no ignition observed on heating under dynamic vacuum <sup>[6]</sup>		
100 °C heat test [% mass loss]	Stability strongly depends on its purity <sup>[3]</sup>		
Vacuum stability test [cm <sup>3</sup> /h]	Stability strongly depends on its purity <sup>[3]</sup>		
Thermal stability	100% dec. occurred @ 72 °C in dry Ar in 43 h <sup>[6]</sup> , 100% dec. occurred @ 72 °C in air with rel. humidity of 87% in 4 h <sup>[6]</sup> , 100% dec. @ RT in air with rel. humidity of 70% in 20 h <sup>[6]</sup>		
Solubility [g/mL]	Easily soluble in water, acetonitrile, alcohols, Et <sub>2</sub> O, ethyl acetate, cyclohexanone, THF, DMSO, nitric acid <sup>[8]</sup> , difficultly soluble in dichloroethane, sulfuric acid <sup>[8]</sup> , insoluble in hexane, CCl <sub>4</sub> <sup>[8]</sup>		
Hygroscopicity	Dec. @ RT in the presence of H <sub>2</sub> O and traces of acids – can lead to spontaneous ignition <sup>[3]</sup> , thermal stability of DNU is very sensitive to air humidity <sup>[6]</sup>		
Compatibility	Dec. @ RT in the presence of H <sub>2</sub> O and traces of acids – can lead to spontaneous ignition <sup>[3]</sup> , quite a strong dibasic acid <sup>[8]</sup> , decomposes in water if a 4× excess of formaldehyde is present <sup>[8]</sup> , decomposes to nitramide if a stoichiometric amount of water is present in an organic solvent <sup>[8]</sup>		
Heat of dec. [cal/g]	475 (exptl.) <sup>[6]</sup> , 455 (calcd.) <sup>[6]</sup> , 2.0 kJ g <sup>-1</sup> (calorimetric) <sup>[6]</sup> , 1.92 kJ g <sup>-1</sup> (calcd.) <sup>[6]</sup>		
Heat of hydrolysis [cal/g]	500 (exptl.) <sup>[6]</sup>		

	<b>DNU<sup>[2,8]</sup></b>
Chemical formula	CH <sub>2</sub> N <sub>4</sub> O <sub>5</sub>
Molecular weight [g mol <sup>-1</sup> ]	150.05
Crystal system	Orthorhombic
Space group	Fdd2
<i>a</i> [Å]	12.0015(9)
<i>b</i> [Å]	17.6425(13)
<i>c</i> [Å]	4.5555(4)
$\alpha$ [°]	90
$\beta$ [°]	90
$\gamma$ [°]	90
<i>V</i> [Å <sup>3</sup> ]	964.57
<i>Z</i>	8
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	2.067
<i>T</i> [K]	90

Single crystals suitable for X-ray diffraction obtained by recryst. from a Et<sub>2</sub>O/hexane mixture<sup>[9]</sup>

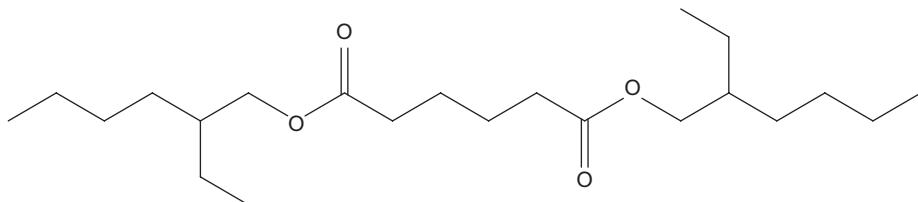
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- [4] L. Liu, K. Dong, X. Yao, Z. Li, C. Li, J. Sun, X. Zhang, S. Zhang, *Combustion and Flame*, **2012**, *159*, 1393–1398.
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## Dioctyl adipate

Name [German, acronym]: Dioctyl adipate, di(2-ethylhexyl) adipate [DOA]

Main (potential) use: Inert plasticizer in gun propellants<sup>[1]</sup>

Structural formula:



	DOA	
Formula	C <sub>22</sub> H <sub>42</sub> O <sub>4</sub>	
Molecular mass [g mol <sup>-1</sup> ]	370.57	
Appearance at RT		
N [%]		
Ω(CO <sub>2</sub> ) [%]	-263.38	
T <sub>m.p.</sub> [°C]	-67.8 <sup>[1]</sup>	
T <sub>b.p.</sub> [°C]	417 <sup>[1]</sup>	
ρ [g cm <sup>-3</sup> ]	0.925 <sup>[1]</sup> , 0.9254 (@ 293.15 K) <sup>[3]</sup> , 0.919 <sup>[4]</sup> , 0.9268 (@ 20 °C) <sup>[5]</sup>	
Heat of formation	-1,215.03 kJ/mol (enthalpy of form.) <sup>[1]</sup> , -3,278.8 kJ/kg (enthalpy of form.) <sup>[1]</sup> , -733 cal/g <sup>[4]</sup>	
	Calcd. (EXPLO5 6.04)	Exptl.
-Δ <sub>ex</sub> U <sup>o</sup> [kJ kg <sup>-1</sup> ]	472	
T <sub>ex</sub> [K]	698	
p <sub>C,J</sub> [GPa]	2.73	
VoD [m s <sup>-1</sup> ]	3,891 (@ 0.925 g cm <sup>-3</sup> , Δ <sub>f</sub> H = -1,214.98 kJ mol <sup>-1</sup> )	
V <sub>0</sub> [L kg <sup>-1</sup> ]	811	

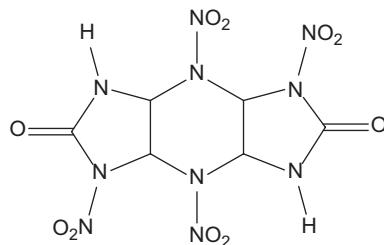
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- [3] J. C. F. Diogo, H. M. N. T. Avelino, F. J. P. Caetano, J. M. N. A. Fareleira, *Fluid Phase Equilibria*, **2014**, 374, 9–19.
- [4] <https://engineering.purdue.edu/~propulsi/propulsion/comb/propellants.html>
- [5] B. T. Fedoroff, O. E. Sheffield, *Encyclopedia of Explosives and Related Items*, vol. 5, US Army Research and Development Command, TACOM, Picatinny Arsenal, USA, **1972**.

**cis-syn-cis-2,6-Dioxo-1,4,7,8-tetranitrodecahydro-1*H*,5*H*-diimidazo[4,5-*b*:4',5'-*e*]pyrazine**

Name [German, acronym]: cis-syn-cis-2,6-Dioxo-1,4,7,8-tetranitrodecahydro-1*H*,5*H*-diimidazo[4,5-*b*:4',5'-*e*]pyrazine, [cis-syn-cis-2,6-dioxo-1,4,7,8-tetranitrodecahydro-1*H*,5*H*-diimidazo[4,5-*b*:4',5'-*e*]pyrazin]

Main (potential) use: secondary explosive

Structural formula:



	<b>cis-syn-cis-2,6-Dioxo-1,4,7,8-tetranitrodecahydro-1<i>H</i>,5<i>H</i>-diimidazo[4,5-<i>b</i>:4',5'-<i>e</i>]pyrazine</b>		
Formula	C <sub>6</sub> H <sub>6</sub> N <sub>10</sub> O <sub>10</sub>		
Molecular mass [g mol <sup>-1</sup> ]	378.17		
Appearance at RT			
<i>N</i> [%]	37.04		
$\Omega(\text{CO}_2)$ [%]	-21.2		
<i>T</i> <sub>m.p.</sub> [°C]	225 <sup>[1]</sup>		
<i>T</i> <sub>dec.</sub> [°C]			
<i>ρ</i> [g cm <sup>-3</sup> ]	1.970 <sup>[1]</sup>		
Heat of formation			
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^{\circ}$ [kJ kg <sup>-1</sup> ]			
<i>T</i> <sub>ex</sub> [K]			
<i>p</i> <sub>C-J</sub> [kbar]			

VoD [ $\text{m s}^{-1}$ ]			
$V_0$ [ $\text{L kg}^{-1}$ ]			
Compatibility	$\text{H}_2\text{O}$ stable <sup>[1]</sup> , very slow dec. in boiling MeOH <sup>[1]</sup>		

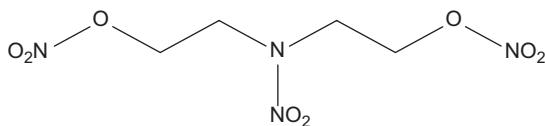
[1] P. F. Pagoria, G. S. Lee, A. R. Mitchell, R. D. Schmidt, *Thermochim. Acta*, **2002**, *384*, 187–204.

## Dioxyethylnitramine dinitrate

Name [German, acronym]: Dioxyethylnitramine dinitrate, bis(nitratoethyl)-nitramine, 2,2'-dinitroxy-diethylnitramine, diethanolnitramine dinitrate, di(2-nitroxyethyl)nitramine, *N,N'*-bis( $\beta$ -nitroxyethyl)-nitramine, 2,2'-(nitroimino)-diethanol dinitrate, ethylene glycol-N-nitramine dinitrate, nitrated ethylene glycol amine, Gina [nitrodiethanolamindinitrat, DINA]

Main (potential) use: Explosive, gelatinizer for nitrocellulose<sup>[27]</sup>, component of double-base propellants<sup>[1]</sup>, propellants<sup>[34]</sup>

Structural formula:



	<b>DINA</b>
Formula	$\text{C}_4\text{H}_8\text{N}_4\text{O}_8$
Molecular mass [g mol <sup>-1</sup> ]	240.13
Appearance at RT	Crystalline solid <sup>[29]</sup> , light yellow crystalline solid <sup>[34]</sup>
IS [J]	6 Nm <sup>[1]</sup> , 23 cm with 2.5 kg hammer <sup>[7]</sup> , 7–12 in (2 kg mass, P.A.) <sup>[9]</sup> , 31 cm (B.M.) <sup>[9]</sup> , drop weight = 7.5 Nm <sup>[15]</sup> , $A_{d1} = 16\%$ , $A_{d2} = 0\%$ , LL = 1.3 m, $A_{50\ d1} = 2.9$ m, $A_{50\ d2} = 4.5$ <sup>[33]</sup> , $H_{84\%} = 25$ cm (10 kg mass) <sup>[34]</sup> , 44 cm (minimum height for detonation, 2 kg mass) <sup>[34]</sup> , 27 cm (ERL #3, sample in brass cup 0.308 in inside diameter, 0.01 in thick, $7/8$ in height, 5 kg mass) <sup>[35]</sup> , 13 cm (ERL #5, sample in cylindrical cavity $1/16$ in deep, 0.376 in inside diameter, 5 kg mass) <sup>[35]</sup> , 23 cm (ERL #12, sample on square of Flint paper, $2^{1/2}$ kg mass) <sup>[35]</sup> , $H_{50\%} = 8$ cm (4 kg mass, B.M. design 5) <sup>[35]</sup> , $H_{50\%} = 71$ cm (5 kg mass, plane sandblasted surfaces) <sup>[35]</sup> , 90 cm (sensitivity to glancing impact, Hercules sliding rod, sandblasted surfaces, 45° slide angle, 10 lb rod, 30 mg sample) <sup>[35]</sup> , $H_{50} = 41.1 \pm 0.03$ cm (type 12, ERL apparatus) <sup>[38]</sup> , $H_{50} = 27$ cm (design no. 3 apparatus) <sup>[40]</sup> , $H_{50} = 47$ cm (design no. 9 apparatus, 2.5 kg hammer) <sup>[40]</sup> , $H_{50} = 25$ cm (design no. 12 apparatus, 33 units cf. TNT = 100 units) <sup>[40]</sup>

	% of explosions in instrument no. 4, K-44-2 drop hammer, 10 kg load, 25 cm drop height, 2 different locations for sample <sup>[37]</sup> :																												
<table border="1" style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th colspan="7" style="text-align: center;">Weight (mg)</th> </tr> <tr> <th colspan="3" style="text-align: center;">Centrally located</th> <th colspan="3" style="text-align: center;">Uniformly located</th> <th></th> </tr> <tr> <th>2</th> <th>15</th> <th>50</th> <th>2</th> <th>10</th> <th>50</th> <th>mg</th> </tr> </thead> <tbody> <tr> <td>16</td> <td>44</td> <td>60</td> <td>4</td> <td>68</td> <td>88</td> <td>%</td> </tr> </tbody> </table>		Weight (mg)							Centrally located			Uniformly located				2	15	50	2	10	50	mg	16	44	60	4	68	88	%
Weight (mg)																													
Centrally located			Uniformly located																										
2	15	50	2	10	50	mg																							
16	44	60	4	68	88	%																							
FS [N]	$p_{fr,LL} = 210 \text{ MPa}$ <sup>[8,33]</sup> , $p_{fr,50\%} = 410 \text{ MPa}$ <sup>[8,33]</sup> , less than PETN <sup>[29]</sup> , lower than PETN but higher than RDX <sup>[34]</sup> , 10% explosion rate with swing angle = 90° and pressure = 39.85 kg/cm <sup>2</sup> <sup>[34]</sup> , $H_{50\%} = 11 \text{ cm}$ (friction pendulum, 30 mg sample, sandblasted surface, 2 in ball, 5 kg weight, 8° angle of incidence) <sup>[35]</sup>																												
N [%]	23.33																												
$\Omega(\text{CO}_2)$ [%]	-26.7																												
$T_{m.p.}$ [°C]	50–51 <sup>[2]</sup> , 52.5 (crystals) <sup>[9]</sup> , 49.5–51.5 <sup>[29,34]</sup> , 52 <sup>[17]</sup> , 52 (Thomas Hoover capillary melting point apparatus @ 2 °C/min) <sup>[23]</sup> , 54–55 <sup>[25]</sup> , 51–52 <sup>[26]</sup>																												
$T_{dec.}$ [°C]	165 <sup>[9]</sup> , 160 begins and vigorously @ 180 <sup>[34]</sup>																												
$\rho$ [g cm <sup>-3</sup> ]	1.488 <sup>[1]</sup> , 1.570 ± 0.06 (@ 293.15 K) <sup>[3]</sup> , 1.67 (@ 25 °C) <sup>[9]</sup> , 1.67 <sup>[25]</sup> , 1.658 (cast charge) <sup>[9]</sup> , 1.488 (pressed @ 3,000 psi) <sup>[9]</sup> , sp. gr. d <sup>15°</sup> <sub>4°</sub> = 1.67 <sup>[29]</sup> , 0.8–0.9 (gravimetric density) <sup>[29]</sup> , 1.67–1.70 <sup>[34]</sup> , 0.8–1.0 (false density) <sup>[34]</sup> , 1.58 (c) <sup>[35]</sup>																												
Heat of formation	-289.1 kJ/mol (enthalpy of form., calcd., S-D method) <sup>[4]</sup> , -221.8 kJ/mol (enthalpy of form., calcd., emp.) <sup>[4]</sup> , -257.4 kJ/mol (enthalpy of form., exptl.) <sup>[4]</sup> , -1,148.2 kJ/kg (enthalpy of form.) <sup>[11]</sup> , -1,133.0 cal/mol ( $\Delta_f H$ ) <sup>[25]</sup> , 282.7 kJ/kg <sup>[28]</sup> , 1,182.82 J/g <sup>[34]</sup> , 1,180.3 (Q <sup>v</sup> ) <sup>[34]</sup> , 283.25 kJ/mol (Q <sup>v</sup> ) <sup>[34]</sup> , 307.5 kJ/mol (Q <sup>p</sup> ) <sup>[34]</sup> , 77.46 kcal/mol (- $\Delta H_f$ (heat of form. @ standard conditions)) <sup>[36]</sup> , -65.88 kcal/mol ( $\Delta H_f^o$ ) <sup>[39]</sup>																												
Heat of combustion	1,260–1,350 cal/g <sup>[9]</sup> , 2,409 kcal/kg (@ C <sup>v</sup> ) <sup>[28]</sup> , 10,079.3 J/g <sup>[34]</sup> , heat of comb. = 573.69 kcal/mol (@ 1 atm) <sup>[35]</sup>																												
Exptl. heat of combustion data <sup>[36]</sup> : <table border="1" style="width: 100%; border-collapse: collapse;"> <tr> <th style="text-align: center;"><math>-\Delta U_{B/M}</math> (cal/g)</th> <th style="text-align: center;"><math>-\Delta U_B</math> (kcal/mol)</th> <th style="text-align: center;"><math>-\Delta U_R</math> (kcal/mol @ 1 atm and constant vol.)</th> <th style="text-align: center;"><math>-\Delta H_R</math> (kcal/mol @ 1 atm and constant pressure)</th> </tr> <tr> <td style="text-align: center;">2,403.18 ± 0.38</td> <td style="text-align: center;">577.09</td> <td style="text-align: center;">576.06</td> <td style="text-align: center;">573.69</td> </tr> </table>		$-\Delta U_{B/M}$ (cal/g)	$-\Delta U_B$ (kcal/mol)	$-\Delta U_R$ (kcal/mol @ 1 atm and constant vol.)	$-\Delta H_R$ (kcal/mol @ 1 atm and constant pressure)	2,403.18 ± 0.38	577.09	576.06	573.69																				
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	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.																										

$-\Delta_{\text{ex}}U^{\circ} [\text{kJ kg}^{-1}]$	5,134	2,960 (calcd.) <sup>[11]</sup> 5,230 (explosion heat) [H <sub>2</sub> O (l)] <sup>[34]</sup>	5,458 [H <sub>2</sub> O (l)] <sup>[1]</sup> 5,025 [H <sub>2</sub> O (g)] <sup>[1]</sup> 1,250 kcal/kg <sup>[29]</sup>
$T_{\text{ex}} [\text{K}]$	3,609	3,450 <sup>[34]</sup>	3,480 <sup>[11]</sup>  3,700 (@ 1.70 g cm <sup>-3</sup> , based on luminosity method data) <sup>[11]</sup>
$p_{\text{CJ}} [\text{GPa}]$	220	217 (calcd.) <sup>[11]</sup>	
VoD [m s <sup>-1</sup> ]	7,426 (@ 1.488 g cm <sup>-3</sup> , Δ <sub>f</sub> H <sup>°</sup> = -329 kJ mol <sup>-1</sup> )	7,469 (@ 1.430 g cm <sup>-3</sup> , calcd.) <sup>[11]</sup>  6,412 (@ 1.0 g cm <sup>-3</sup> , calcd., BKWR) <sup>[12]</sup>  6,163 (@ 1.0 g cm <sup>-3</sup> , calcd., BKWS) <sup>[12]</sup>  7,713 (@ 1.62 g cm <sup>-3</sup> ) <sup>[15]</sup>  7,950 (@ 1.67 g cm <sup>-3</sup> (TMD), calcd., R-P method) <sup>[16]</sup>  8,620 (@ 1.67 g cm <sup>-3</sup> (TMD), calcd., Aizenshtadt method) <sup>[16]</sup>  8,210 (@ 1.67 g cm <sup>-3</sup> (TMD), calcd., K-J) <sup>[16]</sup>  5,950 (@ 1 g cm <sup>-3</sup> , calcd., Kamlet method) <sup>[24]</sup>  7,970 (@ 1.6 g cm <sup>-3</sup> , calcd., Kamlet method) <sup>[24]</sup>  5,350 (@ 1.0 g cm <sup>-3</sup> , calcd., Urizar method) <sup>[24]</sup>	7.80 mm/μs (@ 1.64 g cm <sup>-3</sup> ) <sup>[10,18,24]</sup>  7.72 mm/μs (@ 1.60 g cm <sup>-3</sup> ) <sup>[10,14,18,24]</sup>  7.73 mm/μs (@ 1.60 g cm <sup>-3</sup> ) <sup>[9,18,24]</sup>  7.58 mm/μs (@ 1.55 g cm <sup>-3</sup> ) <sup>[9,18,24]</sup>  7.40 mm/μs (@ 1.48 g cm <sup>-3</sup> ) <sup>[10,24]</sup>  7.00 mm/μs (@ 1.36 g cm <sup>-3</sup> ) <sup>[10,18,24]</sup>  5.80 mm/μs (@ 0.95 g cm <sup>-3</sup> ) <sup>[10,18,24]</sup>  7,580 (@ 1.47 g cm <sup>-3</sup> , confined) <sup>[1]</sup>  8,000 (@ 1.67 g cm <sup>-3</sup> ) <sup>[5,10,24]</sup>  8,000 (@ 1.70 g cm <sup>-3</sup> , based on luminosity method data) <sup>[11]</sup>  5,950 (@ 1.0 g cm <sup>-3</sup> ) <sup>[12,24]</sup>

		7,660 (@ 1.6 g cm <sup>-3</sup> , calcd., Urizar method) <sup>[24]</sup> 7,800 (@ 1.6 g cm <sup>-3</sup> ) <sup>[34]</sup> 7,350 (@ 1.47 g cm <sup>-3</sup> ) <sup>[34]</sup>	7,800 (@ 1.6 g cm <sup>-3</sup> ) <sup>[13]</sup> 23,400 ft/s (@ 1.6 g/mL) <sup>[26]</sup> 7,350 (@ 1.47 g cm <sup>-3</sup> ) <sup>[29]</sup> 7,650 (@ 1.58 g cm <sup>-3</sup> ) <sup>[35]</sup>
$V_0$ [L kg <sup>-1</sup> ]	833	930 (specific volume) <sup>[34]</sup>	924 <sup>[1,6]</sup>
$I_{sp}$ [Ns g <sup>-1</sup> ]	2.56 (calcd., ISPBKW code) <sup>[39]</sup> , 2.55 (calcd., empirical) <sup>[39]</sup>		

Trauzl test [cm <sup>3</sup> , % TNT]	160% TNT <sup>[13]</sup> , 472 <sup>[32]</sup> , 480 <sup>[34]</sup>																															
Lead block compression [mm]	22 ( $H/d = 60/40$ mm) <sup>[34]</sup>																															
Copper column compression [mm]	4.7 <sup>[34]</sup>																															
Sand test [g]	71% TNT <sup>[13]</sup> , 55.3 g sand crushed <sup>[9]</sup>																															
Ballistic mortar test	140–158% TNT <sup>[13]</sup> , 143% TNT <sup>[35]</sup>																															
US NOL gap test	<p>8.39 cm gap value (cast DINA)<sup>[11]</sup></p> <p>Comparison of NOL LSGT results with those of IHE gap test, DINA-c = cast DINA, diameter = 3.65 cm, aspect ratio (<math>l/d</math>) = 2.83, PMMA attenuator, 0.56 cm thick steel confinement<sup>[21]</sup>:</p> <table border="1"> <thead> <tr> <th>Material</th> <th><math>\rho_0</math> (g cm<sup>-3</sup>)</th> <th>LSGT confined (50% gap, in <math>\times 10^2</math>)</th> <th>LSGT unconfined (50% gap, in <math>\times 10^2</math>)</th> </tr> </thead> <tbody> <tr> <td>DINA-c</td> <td>1.60</td> <td>279</td> <td>226</td> </tr> </tbody> </table> <p>Cast DINA (prepared by longitudinal wires and slow cooling), <sup>a</sup> relationship <math>p_i = a + b d^{-1}</math> assumed (TNT Hugoniot was used for DINA), <sup>b</sup> standard LSGT confined charge assumed equivalent to 7.62 cm diameter unconfined charge<sup>[31]</sup>:</p> <table border="1"> <thead> <tr> <th rowspan="2"><math>\rho_0</math> (g cm<sup>-3</sup>)</th> <th rowspan="2"><math>d_e</math> (cm)</th> <th colspan="3">50% point</th> <th rowspan="2">slope<sup>a</sup> <math>\Delta p/\Delta d^{-1}</math> (kbar cm)</th> </tr> <tr> <th>Gap (in <math>\times 10^2</math>)</th> <th><math>p_g</math> (kbar)</th> <th><math>p_i</math> (kbar)</th> </tr> </thead> <tbody> <tr> <td>1.60</td> <td>3.81</td> <td>226</td> <td>15.5</td> <td>17.4</td> <td>49.5</td> </tr> <tr> <td></td> <td>7.62<sup>b</sup></td> <td>279</td> <td>10.0</td> <td>10.9</td> <td></td> </tr> </tbody> </table>			Material	$\rho_0$ (g cm <sup>-3</sup> )	LSGT confined (50% gap, in $\times 10^2$ )	LSGT unconfined (50% gap, in $\times 10^2$ )	DINA-c	1.60	279	226	$\rho_0$ (g cm <sup>-3</sup> )	$d_e$ (cm)	50% point			slope <sup>a</sup> $\Delta p/\Delta d^{-1}$ (kbar cm)	Gap (in $\times 10^2$ )	$p_g$ (kbar)	$p_i$ (kbar)	1.60	3.81	226	15.5	17.4	49.5		7.62 <sup>b</sup>	279	10.0	10.9	
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	7.62 <sup>b</sup>	279	10.0	10.9																												

LSGT [cm]	64 mm (NOL) <sup>[22]</sup>  C = cast; regular tests, all charges conditioned and fired @ 25 °C <sup>[31]</sup> :  <table border="1"> <thead> <tr> <th colspan="2">density</th> <th colspan="2">50% point</th> <th>Particle size (μm)</th> <th>comments</th> </tr> <tr> <th>g/cc</th> <th>% TMD</th> <th>Cards</th> <th>kbar</th> <th></th> <th></th> </tr> </thead> <tbody> <tr> <td>C</td> <td></td> <td>330</td> <td>171</td> <td></td> <td>Ambient <i>T</i>, cream cast</td> </tr> <tr> <td>1.60 C</td> <td>95.8</td> <td>279</td> <td>10</td> <td>249</td> <td>Charge contained</td> </tr> </tbody> </table>	density		50% point		Particle size (μm)	comments	g/cc	% TMD	Cards	kbar			C		330	171		Ambient <i>T</i> , cream cast	1.60 C	95.8	279	10	249	Charge contained
density		50% point		Particle size (μm)	comments																				
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C		330	171		Ambient <i>T</i> , cream cast																				
1.60 C	95.8	279	10	249	Charge contained																				
5 s explosion <i>T</i> [°C] Explosion <i>T</i> [°C] Ignition point [°C]	230 <sup>[34]</sup> 322 <sup>[9]</sup> , 235 <sup>[9]</sup> , 207 (DSC @ 6 °C/min) <sup>[15]</sup> , 200 <sup>[26]+</sup> 240 <sup>[34]</sup>																								
Thermal stability	Begins dec. @ 160 °C and vigorous dec. @ 180 °C <sup>[34]</sup> , thermal stability is very good for pure and dry DINA <sup>[34]</sup> , unstable if triethanolamine impurity is present <sup>[34]</sup> , slower thermal dec. than NG <sup>[34]</sup> , discolored @ 120 °C and showed no epr signal <sup>[41]</sup>																								
100 °C heat test [% mass loss]	0.69% mass loss in first 48 h <sup>[9]</sup> , 0.62% mass loss in second 48 h <sup>[9]</sup> , no explosion in 100 h <sup>[9]</sup>																								
International heat test @ 75 °C	0.4% mass loss in 48 h (U.K.) <sup>[9]</sup> , no loss in 48 h (P.A.) <sup>[9]</sup>																								
Abel heat test	13 min @ 60 °C <sup>[27]</sup> , resistance time = up to 60 min @ 72 °C <sup>[34]</sup>																								
Vacuum stability test [cm <sup>3</sup> /h]	11 + cc gas evolved in 16 h @ 100 °C <sup>[9]</sup> , 10 h, 42 h (time required for >12 cc to be produced @ 100 °C, 2.4 g sample) <sup>[30]</sup>																								
Volatility	0.01% @ 21 °C <sup>[9]</sup> , 0.02% @ 40 °C <sup>[9]</sup> , not volatile <sup>[29]</sup> , 0.7% loss @ 60 °C, 60 h <sup>[34]</sup>																								
Solubility [g/mL]	Soluble in most organic solvents such as acetone, ethyl acetate, Et <sub>2</sub> O, benzene, toluene and CH <sub>2</sub> Cl <sub>2</sub> <sup>[34]</sup> , hardly soluble in CCl <sub>4</sub> , CS <sub>2</sub> or petroleum ether <sup>[34]</sup> , insoluble in water, but becomes slightly soluble on warming <sup>[34]</sup> , 1.0 g/100 g water @ 100 °C <sup>[34]</sup> , very miscible with other nitrates such as NG or EGDN <sup>[34]</sup> , miscible with 98% nitric acid <sup>[34]</sup> , insoluble in hydrochloric acid <sup>[34]</sup>  Solubility of DINA in acetone of different concentrations @ 25 °C <sup>[34]</sup> :  <table border="1"> <thead> <tr> <th>Acetone conc. (%)</th> <th>Dissolved DINA (g)/100 g acetone soln.</th> </tr> </thead> <tbody> <tr> <td>0</td> <td>0.053</td> </tr> <tr> <td>10</td> <td>0.095</td> </tr> <tr> <td>20</td> <td>0.260</td> </tr> <tr> <td>30</td> <td>0.590</td> </tr> <tr> <td>40</td> <td>1.226</td> </tr> <tr> <td>50</td> <td>~ 1.7</td> </tr> <tr> <td>60</td> <td>3.53</td> </tr> <tr> <td>70</td> <td>5.87</td> </tr> <tr> <td>80</td> <td>9.39</td> </tr> </tbody> </table>	Acetone conc. (%)	Dissolved DINA (g)/100 g acetone soln.	0	0.053	10	0.095	20	0.260	30	0.590	40	1.226	50	~ 1.7	60	3.53	70	5.87	80	9.39				
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	<p>Solubility of DINA in 30% acetic acid at different <math>T^{[34]}</math>:</p> <table border="1"> <thead> <tr> <th><math>T</math> (°C)</th><th>20</th><th>25</th><th>30</th><th>40</th></tr> </thead> <tbody> <tr> <td>g DINA/100 g acetic acid</td><td>0.230</td><td>0.353</td><td>0.444</td><td>0.943</td></tr> </tbody> </table> <p>Relation between DINA solubility and acetic acid concentration<sup>[34]</sup>:</p> <table border="1"> <thead> <tr> <th>Acetic acid conc. (%)</th><th>10</th><th>20</th><th>40</th><th>50</th><th>60</th></tr> </thead> <tbody> <tr> <td>g DINA/100 g acetic acid</td><td>0.099</td><td>0.178</td><td>0.729</td><td>1.43</td><td>2.66</td></tr> </tbody> </table> <p>Solubility in water @ different <math>T^{[34]}</math>:</p> <table border="1"> <thead> <tr> <th><math>T</math> (°C)</th><th>20</th><th>25</th><th>30</th><th>40</th><th>60</th><th>100</th></tr> </thead> <tbody> <tr> <td>g DINA/100 g H<sub>2</sub>O</td><td>0.042– 0.05</td><td>0.053</td><td>0.068</td><td>0.129– 0.14</td><td>0.27</td><td>1.0</td></tr> </tbody> </table>	$T$ (°C)	20	25	30	40	g DINA/100 g acetic acid	0.230	0.353	0.444	0.943	Acetic acid conc. (%)	10	20	40	50	60	g DINA/100 g acetic acid	0.099	0.178	0.729	1.43	2.66	$T$ (°C)	20	25	30	40	60	100	g DINA/100 g H <sub>2</sub> O	0.042– 0.05	0.053	0.068	0.129– 0.14	0.27	1.0
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Hygroscopicity	Nonhygroscopic <sup>[26,29]</sup> , does not absorb water @ RT <sup>[34]</sup> , absorbs 0.00375% water @ rel. humidity of 95% @ 40 °C for 8 h <sup>[34]</sup>																																				
Compatibility	Boiling water affects its sensitivity <sup>[26]</sup> , dec. in conc. sulfuric acid even @ 0 °C <sup>[29]</sup> , slow dec. in water (~30% dec. in 6 h) <sup>[29]</sup> , slow dec. by 10% aqueous NaOH soln. <sup>[34]</sup> , dec. on heating in NaOH/EtOH soln. <sup>[34]</sup> , complete dec. in sulfuric acid even @ 0 °C <sup>[34]</sup> , rel. stable in presence of dil. acid and weak reducing agent <sup>[34]</sup> , slower hydrolysis in water cf. NG <sup>[34]</sup> , 3% dec. rate in water @ 80 °C, 2 h <sup>[34]</sup> , 6% dec. rate in water @ 100 °C, 6 h <sup>[34]</sup>																																				
Heat of fusion [kcal/kg]	23.5 <sup>[29]</sup> , 98.32 J/g <sup>[34]</sup>																																				
Specific heat [kcal/kg/°C]	0.38 <sup>[29,34]</sup>																																				
Shooting sensitivity	Explosion rate of 100% <sup>[34]</sup>																																				
Bullet sensitivity	6 (I.I. (ord)) <sup>[35]</sup> , 10 (no I. I. (alz)) <sup>[35]</sup>																																				
Flashpoint [°C]	235 <sup>[37]</sup>																																				

	DINA <sup>[19]</sup>	DINA <sup>[20]</sup>
Chemical formula	C <sub>4</sub> H <sub>8</sub> N <sub>4</sub> O <sub>8</sub>	C <sub>4</sub> H <sub>8</sub> N <sub>4</sub> O <sub>8</sub>
Molecular weight [g mol <sup>-1</sup> ]	240.13	240.13
Crystal system	Orthorhombic	Monoclinic
Space group	Pca21 (no. 29)	P2 <sub>1</sub> /c (no. 14)
$a$ [Å]	15.345(5)	9.06(1)
$b$ [Å]	6.183(2)	9.15(1)
$c$ [Å]	10.095(3)	12.33(2)
$\alpha$ [°]	90	90

$\beta$ [°]	90	109.94(5)
$\gamma$ [°]	90	90
$V$ [Å <sup>3</sup> ]	975.795	960.867
$Z$	4	4
$\rho_{\text{calc}}$ [g cm <sup>-3</sup> ]	1.665	1.66
$T$ [K]	295	295

DINA shows  $\alpha$ - and  $\beta$ -crystalline forms<sup>[34]</sup>

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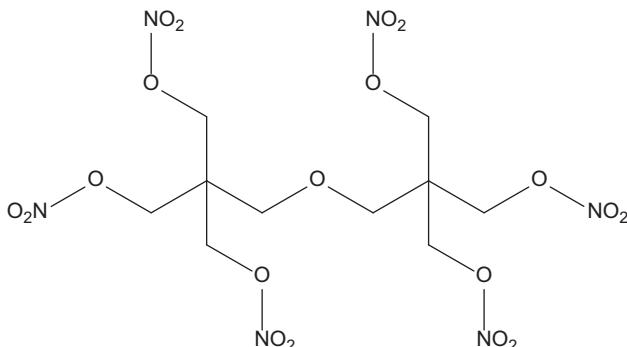
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## Dipentaerythritol hexanitrate

Name [German, acronym]: 2,2'-[Oxybis(methylene)]bis[2-[(nitrooxy)methyl]propane-1,2-diyl] tetranitrate, dipentaerythritol hexanitrate, pentaerythritol hexanitrate, pentaerythrit-2-ol hexanitrate, nitrodipenta, dipenta [hexanitrodipentaerythrit, DIPEHN, DPEHN]

Main (potential) use: Ingredient of primary compositions<sup>[8]</sup>, component of primer or igniter<sup>[22]</sup>

Structural formula:



	DIPEHN
Formula	C <sub>10</sub> H <sub>16</sub> N <sub>6</sub> O <sub>19</sub>
Molecular mass [g mol <sup>-1</sup> ]	524.26
Appearance at RT	White crystals <sup>[16,18]</sup> , white crystals with two crystal forms <sup>[22]</sup>
IS [J]	4 Nm <sup>[1]</sup> , 2.75 (14 cm, 2 kg mass, 20 mg sample, B. M.) <sup>[8]</sup> , 1.99 (4 in, 2 kg mass, 10 mg sample, P.A.) <sup>[8]</sup> , 14 cm (2 kg mass, B.M.) <sup>[11]</sup> , 4 in (2 kg mass, 10 mg sample, P.A.) <sup>[11]</sup> , H <sub>50%</sub> = 37 cm (Bruceton no. 3 apparatus) <sup>[11]</sup> , 0/6 shots @ 20 cm, 1/6 shots @ 22 cm (Kast apparatus) <sup>[11]</sup> , less sensitive than PETN <sup>[15]</sup> , 20 ± 0.02 cm (type 12A) <sup>[23]</sup> , 25 ± 0.07 cm (type 12B) <sup>[23]</sup>
FS [N]	Less sensitive than PETN <sup>[15]</sup> , explodes with steel shoe (friction pendulum test) <sup>[8]</sup> , unaffected by fiber shoe (friction pendulum test) <sup>[8]</sup>
N [%]	16.03
Ω(CO <sub>2</sub> ) [%]	-27.5
T <sub>phase transition</sub> [°C]	Dimorphic: form I = stable modification @ RT, can be grown as dendrites from supercooled melt, large crystals of form II can be grown from melt <70 °C <sup>[21]</sup>

$T_{\text{m.p.}}$ [°C]	75 (polymorph I) <sup>[2]</sup> , 72.5 (polymorph II) <sup>[2]</sup> , 73.5 <sup>[8]</sup> , 73.7–75 <sup>[11]</sup> , 72 <sup>[15,16]</sup> , 71.5 (onset), 73.1 (peak max), 74.7 (end $T$ ) (DSC @ 10.0 K/min, pinhole cover) <sup>[17]</sup> , 73.7 <sup>[8]</sup> 72 (pure) <sup>[8]</sup> , 76 (form I, hot stage microscopy) <sup>[21]</sup> , 74.4 (form II, hot stage microscopy) <sup>[21]</sup> , 75 (stable crystal form) <sup>[22]</sup> , 72.5 (unstable crystal form) <sup>[22]</sup> , 75 (recryst. from EtOH) <sup>[23]</sup> , 71.5 (endo, onset), 73.1 (endo, peak max) (DSC 10 K/min) <sup>[27]</sup>						
$T_{\text{dec.}}$ [°C]	191.6 <sup>[3]</sup> , (explodes >250 <sup>[11]</sup> ), 191.6 (onset), 210.8 (peak max), 220.3 (end $T$ ) (DSC @ 10.0 K/min, pinhole cover) <sup>[17]</sup> , 191.6 (exo, onset), 210.8 (exo, peak max) (DSC 10 K/min) <sup>[27]</sup>						
Nonisothermal TG data <sup>[27]</sup> :							
$\beta$ (K min <sup>-1</sup> )	$T_{\text{ot}}$	$T_i$	Mass loss(%)		$L_{\text{max}}$ (% min <sup>-1</sup> )	$T_p$ (°C)	$T_{\text{oe}}$ (°C)
			Stage 85.981	Residue(%)			
5.0	180.2	162.7	88.15	1.55	-19.03	193.2	227.4
7.0	183.6	163.6	85.98	5.85	-25.53	197.0	230.9
10.0	187.8	164.9	85.14	8.44	-37.17	201.4	236.1
15.0	192.2	166.7	88.6173	10.93	-56.35	206.3	244.8
$T_{\text{ot}} = \text{onset } T \text{ of dec., } T_{\text{oe}} = \text{onset } T \text{ of end of dec., } T_i = \text{initial } T \text{ for thermal dec.,}$ $T_p = \text{peak } T \text{ of mass loss rate, stage 1 = from initial } T \text{ to end } T \text{ of DTG peak,}$ $L_{\text{max}} = \text{max. mass loss rate}$							
$\rho$ [g cm <sup>-3</sup> ]	1.664 ± 0.06 (@ 293.15 K) <sup>[4]</sup> , 1.613 (@ 15 °C, cast) <sup>[11]</sup> , 1.63 <sup>[8,22]</sup> , 1.59 (loading $\rho$ @ 3,000–4,000 kpsi) <sup>[8,11]</sup> , 1.51 (loading $\rho$ of pressed @ 2,000 kg/sq cm) <sup>[11]</sup> , 1.63 (sp. gr., crystals @ 15 °C) <sup>[11]</sup> , sp. gr. = 1.630 @ 15 °C (crystals) <sup>[15]</sup> , sp. gr. = 1.589 (pellets prepared under pressure of 2,500 kg/cm <sup>2</sup> ) <sup>[15]</sup> , 1.613 (after being fused and solidified @ 15 °C) <sup>[16]</sup> , 1.63 (crystal) <sup>[8]</sup>						
Heat of formation	-975.3 kJ/mol (enthalpy of form., calcd., S-D method) <sup>[5]</sup> , -923.8 kJ/mol (enthalpy of form., calcd., emp.) <sup>[5]</sup> , -979.5 kJ/mol (enthalpy of form., exptl.) <sup>[5]</sup> , -1867 kJ/kg (enthalpy of form.) <sup>[1]</sup> , 389.5 kcal/kg <sup>[19]</sup> , 226.7 kcal/mol (@ C) <sup>[11]</sup> , 238.6 kcal/mol (@ C <sup>p</sup> ) <sup>[11]</sup> , 236.32 kcal/mol (-ΔH <sub>f</sub> (heat of form. @ standard conditions)) <sup>[24]</sup> , -233.79 kcal/mol (ΔH <sub>f</sub> <sup>o</sup> ) <sup>[25]</sup> , -979.6 ± 5.4 kJ/mol (ΔH <sub>f</sub> <sup>o</sup> , (c)) <sup>[26]</sup>						
Heat of combustion	2,260 kcal/kg <sup>[8,11,14]</sup> , 1,258.4 kcal/mol <sup>[11]</sup> , 2,434 kcal/kg @ C <sup>v</sup> <sup>[19]</sup> , 5,250.0 kJ/mol (ΔH <sub>c</sub> , heat of comb.) <sup>[27]</sup>						
exptl. heat of combustion data <sup>[24]</sup> :							
$-\Delta U_{B/M}$ (cal/g)	$-\Delta U_B$ (kcal/mol)	$-\Delta U_R$ (kcal/mol @ 1 atm and constant vol.)	$-\Delta H_R$ (kcal/mol @ 1 atm and constant pressure)				
2,407.81 ± 1.38	1,262.36	1,259.98	1,254.94				

	Calcd. (EXPLO5 6.04)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^\circ$ [kJ kg <sup>-1</sup> ]		5,149 (calcd., K-J) <sup>[6]</sup>	5,143 [H <sub>2</sub> O (l)] <sup>[1]</sup> 4,740 [H <sub>2</sub> O (g)] <sup>[1]</sup> 5,143 <sup>[6]</sup> 5,208 <sup>[10]</sup> Heat of detonation = 1,092 cal/g <sup>[11]</sup>
$T_{\text{ex}}$ [K]		3,240 <sup>[12]</sup>	3,240 <sup>[11]</sup>
$p_{\text{C-J}}$ [GPa]			
VoD [m s <sup>-1</sup> ]		7,930 (@ 1.488 g cm <sup>-3</sup> , calcd. K-J) <sup>[3,17]</sup>  7,550 (@ 1.63 g cm <sup>-3</sup> (TMD), calcd., R-P method) <sup>[13]</sup>	7,400 (@ 1.6 g cm <sup>-3</sup> , confined) <sup>[1]</sup> 7,530 (@ 1.63 g cm <sup>-3</sup> , confined) <sup>[7]</sup> 7,410 (@ 1.59 g cm <sup>-3</sup> , 0.39 in charge diameter, pressed, Cu tube confinement) <sup>[8]</sup> 7,450 (@ 1.63 g cm <sup>-3</sup> ) <sup>[12]</sup> 7,410 (@ sp. gr. = 1.59) <sup>[11]</sup> 7,410 (@ sp. gr. = 1.589) <sup>[15]</sup> 7,370 (@ 1.589 g cm <sup>-3</sup> , Dautriche method, Cu tubes, 10 mm diameter, compressed under 2,500 kg cm <sup>2</sup> ) <sup>[16]</sup> 7,450 (@ 1.589 g cm <sup>-3</sup> , Dautriche method, Cu tubes, 10 mm diameter, compressed under 2,500 kg cm <sup>2</sup> ) <sup>[16]</sup>
$V_0$ [L kg <sup>-1</sup> ]			
$I_{\text{sp}}$ [NS g <sup>-1</sup> ]		2.49 (calcd., ISPBKW code) <sup>[25]</sup> , 2.46 (calcd., empirical) <sup>[25]</sup>	

Trauzl test [cm <sup>3</sup> , % TNT]	128% TNT <sup>[8,12]</sup> , 380 cc (cf. 295 cc for TNT) <sup>[11]</sup> , 128% TNT <sup>[11]</sup> , 75% PETN <sup>[15]</sup> , 283 cc (10 g sample) <sup>[16]</sup> , 380 cm <sup>3</sup> <sup>[20]</sup>
Sand test [g]	119% TNT <sup>[12]</sup> , 57.4 g sand crushed (200 g bomb, 0.4 g sample initiated by LA, cf. 62.7 g sand crushed by PETN) <sup>[11]</sup> , 57.4 g (200 g bomb) <sup>[8]</sup>

Ballistic mortar test	144% TNT <sup>[11,12]</sup> , 142% TNT <sup>[8,11]</sup>																									
5 s explosion $T$ [°C]	255 <sup>[8,11]</sup>																									
1 s explosion $T$ [°C]	300 <sup>[8,11]</sup>																									
5 s ignition $T$ [°C]	255 (explodes, US value) <sup>[14]</sup> , 255 (Russian value) <sup>[14]</sup>																									
100 °C heat test [% mass loss]	0.11% mass loss in first 48 h <sup>[8,11]</sup> , 0.10% mass loss in second 48 h <sup>[8,11]</sup> , no explosion in 100 h <sup>[8,11]</sup>																									
Thermal stability	<p>Nonisothermal TG data, <math>\beta = {}^\circ\text{C}/\text{min}</math>, <math>T_{\text{ei}}</math> = onset <math>T</math> of TG peaks, <math>T_p</math> = peak <math>T</math>, <math>T_{\text{oe}}</math> = endset <math>T</math> of TG peaks, <math>T_b</math> = critical <math>T</math> for thermal dec.<sup>[17]</sup>:</p> <table border="1"> <thead> <tr> <th><math>\beta</math> (°C/min)</th> <th><math>T_{\text{ei}}</math> (°C)</th> <th><math>T_p</math> (°C)</th> <th><math>T_{\text{oe}}</math> (°C)</th> <th><math>T_b</math> (°C)</th> </tr> </thead> <tbody> <tr> <td>5.0</td> <td>180.2</td> <td>193.2</td> <td>227.4</td> <td>181.8</td> </tr> <tr> <td>7.0</td> <td>183.6</td> <td>197.0</td> <td>230.9</td> <td></td> </tr> <tr> <td>10.0</td> <td>187.8</td> <td>201.4</td> <td>236.1</td> <td></td> </tr> <tr> <td>15.0</td> <td>192.2</td> <td>206.3</td> <td>244.8</td> <td></td> </tr> </tbody> </table> <p>Critical <math>T</math> for thermal dec. = 181.8 °C<sup>[27]</sup></p>	$\beta$ (°C/min)	$T_{\text{ei}}$ (°C)	$T_p$ (°C)	$T_{\text{oe}}$ (°C)	$T_b$ (°C)	5.0	180.2	193.2	227.4	181.8	7.0	183.6	197.0	230.9		10.0	187.8	201.4	236.1		15.0	192.2	206.3	244.8	
$\beta$ (°C/min)	$T_{\text{ei}}$ (°C)	$T_p$ (°C)	$T_{\text{oe}}$ (°C)	$T_b$ (°C)																						
5.0	180.2	193.2	227.4	181.8																						
7.0	183.6	197.0	230.9																							
10.0	187.8	201.4	236.1																							
15.0	192.2	206.3	244.8																							
Vacuum stability test [cm <sup>3</sup> /h]	3.7 cc/40 h (@ 100 °C) <sup>[8,11]</sup> , 11 + cc/40 h (@ 120 °C) <sup>[8,11]</sup>																									
Solubility [g/mL]	Soluble in acetone <sup>[15]</sup> , more soluble in acetone than PETN <sup>[22]</sup> , more soluble in conc. nitric acid than PETN <sup>[22]</sup> , extremely soluble in acetone <sup>[23]</sup> , recryst. from EtOH <sup>[23]</sup>																									
Hygroscopicity	0.03% <sup>[8]</sup>																									
$\Delta H_{\text{melt}}$ [J/g]	-214.7 (heat absorption) <sup>[17]</sup>																									
$\Delta H_{\text{dec.}}$ [J/g]	4,678 (heat release) <sup>[17]</sup> , 1,413.2 kJ/mol ( $\Delta H_d$ , heat of dec.) <sup>[27]</sup>																									

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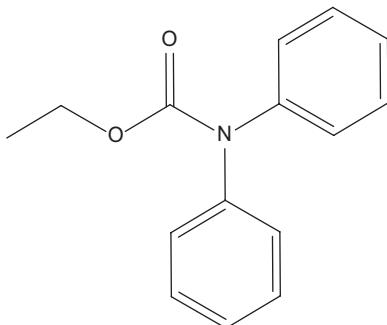
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## Diphenylurethane

Name [German, acronym]: Diphenylurethane [diphenylurethan]

Main (potential) use: Gunpowder stabilizer, gelatinizer<sup>[1]</sup>

Structural formula:



	Diphenylurethane	
Formula	C <sub>15</sub> H <sub>15</sub> NO <sub>2</sub>	
Molecular mass [g mol <sup>-1</sup> ]	241.29	
N [%]	5.81	
Ω(CO <sub>2</sub> ) [%]	-235.4	
T <sub>m,p.</sub> [°C]	72 <sup>[1,2]</sup>	
ρ [g cm <sup>-3</sup> ]	1.146 ± 0.06 (@ 293.15 K) <sup>[3]</sup>	
Heat of formation	-280.7 kJ/mol (Δ <sub>f</sub> H <sup>o</sup> ) <sup>[1]</sup> , -1,163.5 kJ/kg (Δ <sub>f</sub> H <sup>o</sup> ) <sup>[1]</sup>	
	Calcd. (K-J)	Exptl.
-Δ <sub>ex</sub> U <sup>o</sup> [kJ kg <sup>-1</sup> ]		
T <sub>ex</sub> [K]		
p <sub>C-J</sub> [GPa]		
VoD [m s <sup>-1</sup> ]		
V <sub>0</sub> [L kg <sup>-1</sup> ]		

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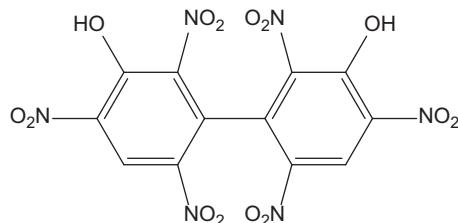
[3] Calculated using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994–2017 ACD/Labs).

## Dipicric acid

Name [German, acronym]: 3,3'-Dihydroxy-2,2',4,4'6,6'-hexanitrobiphenyl,  
[dipikrinsäure, DIPA]

Main (potential) use: Possible thermally stable booster explosive<sup>[1]</sup>

Structural formula:



	DIPA		
Formula	$C_{12}H_4N_6O_{14}$		
Molecular mass [g mol <sup>-1</sup> ]	456.19		
Appearance at RT	Colorless needles (from benzene) <sup>[1]</sup> , yellow amorphous solid (crude DIPA) <sup>[1]</sup>		
IS [J]	42 cm <sup>[1]</sup>		
N [%]	18.42		
$\Omega(CO_2)$ [%]	-42.1		
$T_{m.p.}$ [°C]	311–312 (dec., pure sample) <sup>[1]</sup> , 301 (dec.) <sup>[1]</sup>		
$T_{dec.}$ [°C]	311–312 <sup>[1]</sup>		
$\rho$ [g cm <sup>-3</sup> ]	1.82 (crystal) <sup>[1]</sup>		
Heat of formation			
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{ex}U^o$ [kJ kg <sup>-1</sup> ]			
$T_{ex}$ [K]			
$p_{C,J}$ [kbar]			
VoD [m s <sup>-1</sup> ]			
$V_0$ [L kg <sup>-1</sup> ]			

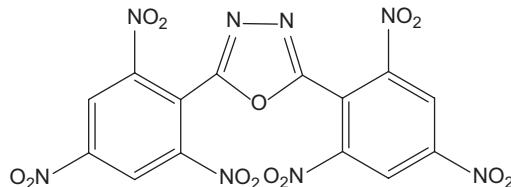
Thermal stability	5.6 cc/g/h gas evolved @ 260 °C <sup>[1]</sup> , 1.8 cc/g/h gas evolved @ 230 °C <sup>[1]</sup>
Solubility [g/mL]	Soluble in H <sub>2</sub> O, MeOH, MeCN <sup>[1]</sup> , highly soluble in water <sup>[1]</sup> , very soluble in H <sub>2</sub> O, EtOH, acetone and acetic acid <sup>[1]</sup> , difficultly: soluble in Et <sub>2</sub> O, benzene, CHCl <sub>3</sub> , conc. HCl <sup>[1]</sup>
Hygroscopicity	Turns yellow in moist air <sup>[1]</sup>
Compatibility	Expected to be corrosive with metals (high pK <sub>a</sub> and H <sub>2</sub> O solubility) <sup>[1]</sup>
pK <sub>a</sub>	~0.5 <sup>[1]</sup>

- [1] H. G. Adolph, J. C. Dacons, M. J. Kamlet, *Heat Resistant Explosives, XI. An Unusual Oxidation Reaction Leading to 3,3'-Dihydroxy-2,2'4,4',6,6'-Hexanitrobiphenyl (Dipicric Acid, DPA)*, NOLTR 62-32, US Naval Ordnance Laboratory, White Oak, USA, 26th February 1962.

## 2,5-Dipicryl-1,3,4-oxadiazole

Name [German, acronym]: Dipicryloxadiazole, [2,5-dipikryl-1,3,4-oxadiazol, DPO]  
 Main (potential) use: Possible future substitute for PETN<sup>[1]</sup>, high temperature downhole explosive<sup>[2]</sup>

Structural formula:



	DPO		
Formula	$\text{C}_{14}\text{H}_4\text{N}_8\text{O}_{13}$		
Molecular mass [g mol <sup>-1</sup> ]	492.23		
Appearance at RT			
IS [J]	20 cm (type 12 tool, 2.5 kg mass, ERL machine) <sup>[1]</sup> , 20 cm <sup>[2]</sup>		
N [%]	22.77		
$\Omega(\text{CO}_2)$ [%]	-55.3		
$T_{\text{m.p.}}$ [°C]	310–311 <sup>[1]</sup> , 335 (high purity, recryst. from acetone-MeOH, vigorous dec.) <sup>[1]</sup>		
$T_{\text{dec.}}$ [°C]			
$\rho$ [g cm <sup>-3</sup> ]	1.77 (crystal, flotation method) <sup>[1]</sup>		
Heat of formation			
	Calcd. (EXPLO5 6.03)	Lit. values	Exptl.
$-\Delta_{\text{ex}}U^\circ$ [kJ kg <sup>-1</sup> ]			
$T_{\text{ex}}$ [K]			
$p_{\text{C.J}}$ [kbar]			
VoD [m s <sup>-1</sup> ]			
$V_0$ [L kg <sup>-1</sup> ]			

Vacuum stability test [cm <sup>3</sup> /h]	0.6 cc/g/h (2 h period) @ 260 °C <sup>[12]</sup>
Solubility [g/mL]	Essentially insoluble in dichloroethane <sup>[1]</sup> , soluble in γ-butyrolactone (1 g/5 mL @ 100 °C) <sup>[1]</sup> , soluble in DMF <sup>[1]</sup>
Shock sensitivity	Short pulse shock tests (exploding foil): threshold flyer velocity = 2.33 km/s, $\rho = 1.61 \text{ g cm}^{-3}$ , consolidation pressure = 103.4 MPa <sup>[1]</sup>

[1] M. E. Sitzmann, *J. Energet. Mater.*, **1988**, 6, 129–144.

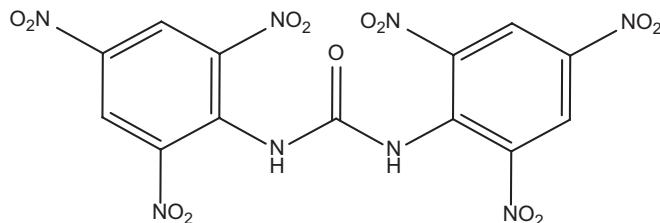
[2] W. Yang, R. A. Parrott, L. A. Behrmann, W. E. Voreck, P. Kneisel, *High Temperature Explosives for Downhole Well Applications*, US Patent US 2002/0129940 A1, 19th September 2002.

## Dipicrylurea

Name [German, acronym]: Dipicrylurea, hexanitrodiphenylurea, hexanitrocarbanilide, *sym*-dipicryl urea, 2,2',4,4',6,6'-hexanitro-*N,N'*-diphenylurea, [hexanitrocarbanilid]

Main (potential) use: High explosive, possible use in boosters, primer caps, no uses since it is susceptible to hydrolysis<sup>[3]</sup>, brisant high explosive can be used in boosters, reinforced detonators, detonating fuse, primer caps<sup>[5]</sup>

Structural formula:



	Dipicrylurea
Formula	C <sub>13</sub> H <sub>6</sub> N <sub>8</sub> O <sub>13</sub>
Molecular mass [g mol <sup>-1</sup> ]	482.23
Appearance at RT	Pale yellow crystals <sup>[3]</sup> , pale yellow rosettes if recryst. from acetone-ligroin <sup>[5]</sup>
IS [J]	Similar to tetryl <sup>[1]</sup>
N [%]	23.24
Ω(CO <sub>2</sub> ) [%]	-53.1
T <sub>m.p.</sub> [°C]	203 <sup>[1]</sup> , 208–209 (with dec.) <sup>[3]</sup> , 204 (pale yellow rosettes obtained from recryst. from acetone-ligroin soften and darken) <sup>[5]</sup> , 208–209 (pale yellow rosettes obtained from recryst. from acetone-ligroin, melt with dec.) <sup>[5]</sup>
T <sub>dec.</sub> [°C]	
ρ [g cm <sup>-3</sup> ]	2.001 ± 0.06 (@ 293.15 K) <sup>[2]</sup>
Heat of formation	
	Calcd. (K-J)
	Exptl.

$-\Delta_{\text{ex}} U^{\circ} [\text{kJ kg}^{-1}]$		
$T_{\text{ex}} [\text{K}]$		
$p_{\text{C-J}} [\text{GPa}]$		
$\text{VoD} [\text{m s}^{-1}]$		
$V_0 [\text{L kg}^{-1}]$		

Sand test [g]	84% TNT <sup>[4]</sup>
Ballistic mortar test	76% TNT <sup>[4]</sup>
Initiation efficiency	Detonation of 0.4 g requires 0.19 g MF <sup>[5]</sup>
5 s explosion $T [\text{°C}]$	
Initiation $T [\text{°C}]$	345 <sup>[3]</sup>
Explosion $T [\text{°C}]$	345 <sup>[5]</sup>

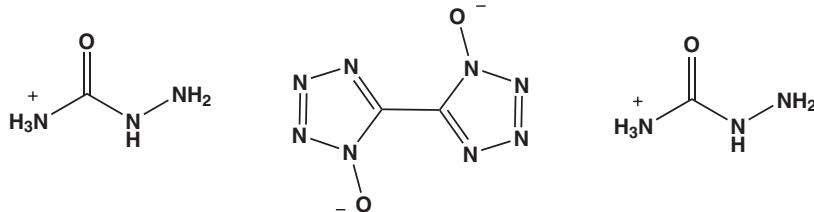
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- [3] T. Urbanski, *Nitro Derivatives of Aniline*, Ch. 17 in *Chemistry and Technology of Explosives*, vol. 1, Pergamon Press, Oxford, **1964**.
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- [5] T. L. Davis, *The Chemistry of Powder and Explosives*, vol. 1, **1941**, John Wiley and Sons Inc., New York, pp. 188–189.

**Di(semicarbazide) 5,5'-bitetrazole-1,1'-diolate**

Name [German, acronym]: Di(semicarbazide) 5,5'-bitetrazole-1,1-diolate

Main (potential) use: Secondary explosive

Structural formula:



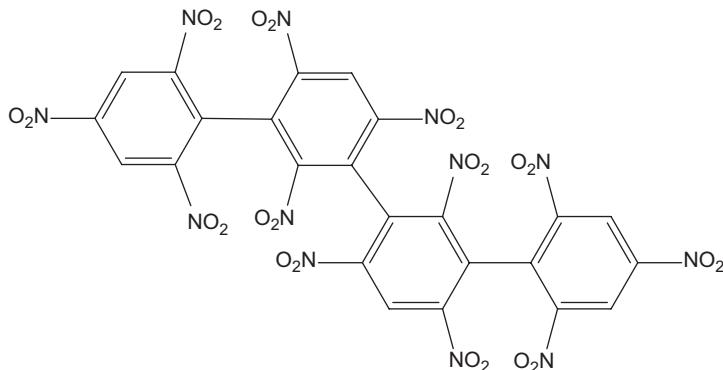
	2SCZ.BTO	
Formula	$C_4H_{12}N_{14}O_4$ , $[CH_6N_3O]^{+}_2 [C_2N_8O_2]^{2-}$	
Molecular mass [g mol <sup>-1</sup> ]	320.28	
Appearance at RT		
IS [J]	25	
N [%]	61.32	
$\Omega(CO_2)$ [%]	-49.9	
$T_{dec.}$ [°C]	239 (DSC @ 5 °C/min)	
$\rho$ [g cm <sup>-3</sup> ]	1.685 (@ 298 K)	
Heat of formation	158.1 kJ/mol ( $\Delta_f H^\circ$ )	
	Calcd. (K-J)	Exptl.
$-\Delta_{ex}U^\circ$ [kJ kg <sup>-1</sup> ]		
$T_{ex}$ [K]		
$p_{C,J}$ [kbar]	235	
VoD [m s <sup>-1</sup> ]	7,433 (@ TMD)	
$V_0$ [L kg <sup>-1</sup> ]		

## 2,2',2'',2''',4,4',4'',4''',6,6',6'',6'''-Dodecanitroquaterphenyl

Name [German, acronym]: 2,2',2'',2''',4,4',4'',4''',6,6',6'',6'''-Dodecanitroquatraphenyl,  
 2,2',2'',2''',4,4',4'',4''',6,6',6'',6'''-dodecanitro-  
 1,1':3'1"3",1'''-quaterphenyl,  
 2,2',2'',2''',4,4',4'',4''',6,6',6'',6'''-dodecanitro-[1, 3'1', 1"]  
 quaterphenyl [DODECA]

Main (potential) use: High thermal stability secondary explosive, component  
 of perforators or detonators in downhole well  
 applications, possible spacecraft applications<sup>[4]</sup>

Structural formula:



	<b>DODECA</b>
Formula	C <sub>24</sub> H <sub>6</sub> N <sub>12</sub> O <sub>24</sub>
Molecular mass [g mol <sup>-1</sup> ]	846.37
Appearance at RT	
IS [J]	H <sub>50%</sub> = 31 cm (recryst. from acetone/toluene, ERL, 2.5 kg mass, sandpaper) <sup>[2]</sup> , H <sub>50%</sub> = 35 cm (recryst. from acetone/acetic acid, ERL, 2.5 kg mass, sandpaper) <sup>[2]</sup> , 9.85 (Bruceton method) <sup>[5,9]</sup> , H <sub>50</sub> = 40 cm (2.5 kg mass, type 12 tool) <sup>[7]</sup>
N [%]	19.86
Ω(CO <sub>2</sub> ) [%]	-51.0
T <sub>m.p.</sub> [°C]	>425 <sup>[3]</sup> , >425 (Thomas Hoover capillary melting point apparatus @ 2 °C/min) <sup>[6]</sup>
T <sub>dec.</sub> [°C]	
ρ [g cm <sup>-3</sup> ]	1.81 (crystal) <sup>[1]</sup>

Heat of formation	50.6 kcal mol <sup>-1</sup> ( $\Delta_f H^\circ$ ) <sup>[1,12]</sup> , 213.0 kJ/mol (enthalpy of form., exptl.) <sup>[11]</sup> , 201.1 kJ/mol (enthalpy of form., calcd., emp.) <sup>[11]</sup> , 229.1 kJ/mol (enthalpy of form., calcd., S-D method) <sup>[11]</sup> , 213 ± 10 kJ/mol ( $\Delta_f H^\circ$ solid) <sup>[13]</sup>		
Heat of combustion	-2,512.8 kcal mol <sup>-1</sup> ( $\Delta_c H$ ) <sup>[1,12]</sup> , -10,515 ± 4 kJ/mol ( $\Delta_c H^\circ$ solid) <sup>[13]</sup>		
	Calcd. (EXPLO5 6.04)	Literature	Exptl.
-Δ <sub>ex</sub> U° [kJ kg <sup>-1</sup> ]		$Q_{\text{real}} = 4,802 \text{ MJ kg}^{-1}$ (@ TMD, calcd., K-J) <sup>[5,9]</sup>	
T <sub>ex</sub> [K]			
p <sub>C-J</sub> [kbar]		264 (calcd. K-J) <sup>[1]</sup>	
VoD [m s <sup>-1</sup> ]		7,700 (@ 1.81 g cm <sup>-3</sup> ) <sup>[1]</sup>  7,690 (@ TMD, calcd., K-J) <sup>[5,9]</sup>	
V <sub>0</sub> [L kg <sup>-1</sup> ]			
Thermal stability	270 °C (threshold of thermal stability) <sup>[5]</sup>		
Vacuum stability test [cm <sup>3</sup> /h]	@ 260 °C (recryst. from acetone/toluene, bulk ρ = 0.28 g/cc): 20 min. surge – 0.43 cc/g gas released; 0.58 cc/g/2 h.; 0.54 cc/g/24 h. <sup>[2]</sup> @ 260 °C (recryst. from acetone/benzene, bulk ρ = 0.31 g/cc): 20 min. surge – 0.64 cc/g gas released; 0.67 cc/g/2 h.; 0.74 cc/g/24 h. <sup>[2]</sup> @ 260 °C (recryst. from acetone/CH <sub>3</sub> CN, bulk ρ = 0.16 g/cc): 20 min. surge – 0.90 cc/g gas released; 0.87 cc/g/2 h.; 0.85 cc/g/24 h. <sup>[2]</sup> @ 260 °C (recryst. from acetone/acetic acid, bulk ρ = 0.26 g/cc): 20 min. surge – 0.47 cc/g gas released; 0.44 cc/g/2 h.; 0.37 cc/g/24 h. <sup>[2]</sup> @ 200 °C, total gas evolved (cm <sup>3</sup> /g) @ STP/time of exposure (days): 0.9/2, 1.4/7, 1.9/14, 2.4/21, 2.9/28, 3.5/35, 4.2/42, 6.3/49, 7.1/56, 7.7/63, 8.0/70, 8.4/77, 9.0/84, 9.7/91 <sup>[8]</sup> @ 175 °C, total gas evolved (cm <sup>3</sup> /g) @ STP/time of exposure (days): 0.5/2, 0.7/7, 0.8/14, 0.9/21, 0.9/28, 0.9/35, 1.0/42, 1.0/49, 1.0/56, 1.1/63, 1.2/70, 1.3/77, 1.4/84, 1.4/91 <sup>[10]</sup>		

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