Supplementary information

Current Trends in Analytical Methods for Determination of Explosives in Water

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Table S1. Overview of nitro-compounds and explosives and their properties

Nitro compound Explosive	Name of the nitro compound or explosive	Molecular formula	Molar mass (g/mol)	Melting point (°C)	Boiling point (°C)	Water solubility at 25 °C (mg/l)	logP
NB	Nitrobenzene	$C_6H_5NO_2$	123.11	5.85	210.9	1900	1.85
1,2-DNB	1,2-Dinitrobenzene	$C_6H_4N_2O_4$	168.11	118	318	1300	1.69
1,2-DNG	1,2-Dinitroglycerin	$C_3H_6N_2O_7$	182.09	FP: 55.3	167.9	140	0.83
1,3,5-TNB	1,3,5-Trinitrobenzene	$C_6H_3N_3O_6$	213.105	123.2	315	330	
1,3-DNB	1,3-Dinitrobenzene	$C_6H_4N_2O_4$	168.11	90	291	500	1.49
1,3-DNG	1,3-Dinitroglycerin	$C_3H_6N_2O_7$	182.09	26	FP: 56.8	72 700	0.71
1,3-DNN	1,3-Dinitronaphthalene	$C_{10}H_6N_2O_4$	218.17	146-148	sublimes	less than 1000	2.83
1,4-DNB	1,4-Dinitrobenzene	$C_6H_4N_2O_4$	168.11	174	297	69	1.46
1,4-DNN	1,4-Dinitronaphthalene	$C_{10}H_6N_2O_4$	218.17	134	386.1	< 1	3.0
1,6-DNN	1,6-Dinitronaphthalene	$C_{10}H_6N_2O_4$	218.17	214 – 218	401.5	< 1	3.7
1,8-DNN	1,8-Dinitronaphthalene	$C_{10}H_6N_2O_4$	218.17	173	sublimes	< 1000	2.5
1-Cl-2,4-DNB	1-Chloro-2,4-dinitrobenzene	$C_6H_3ClN_2O_4$	202.55	53	315	9.24	2.17
1-Cl-2-NB	1-Chloro-2-nitrobenzene	$C_6H_4ClNO_2$	157.55	32.5	245.5	441	2.2
1-Cl-3-NB	1-Chloro-3-nitrobenzene	$C_6H_4ClNO_2$	157.55	46	236	237	2.5
1-Cl-4-NB	1-Chloro-4-nitrobenzene	$C_6H_4ClNO_2$	157.55	182.5	242	< 1000	2.4
1-NN	1-Nitronaphthalene	$C_{10}H_7NO_2$	173.17	61	304	< 1000	3.19
2,3-DNT	2,3-Dinitrotoluene	$C_7H_6N_2O_4$	182.13	60	284	161	1.9
2,4,6-TNP	2,4,6-Trinitrophenol picric acid	$C_6H_3N_3O_7$	229.1	122.5	>300	12 700	1.83

2,4-CNT	2,4-Chloronitrotoluene	$C_7H_6ClNO_2$	171.58	68	260	49	3.08
2,4-DA-6-NT	2,4-Diamino-6-nitrotoluene	$C_7H_9N_3O_2$	167.17	135	406.7	< 10	0.6
2,4-DNCB	2,4-Dinitrochlorobenzene	$C_6H_3ClN_2O_4$	202.55	53	315	9.24	2.3
2,4-DNP	2,4-Dinitrophenol	$C_6H_4N_2O_5$	184.11	115.5	sublimes	2790	1.67
2,4-DNT	2,4-Dinitrotoluene	$C_7H_6N_2O_4$	182.134	70	300	200	1.98
2,5-DCNB	2,5-Dichloronitrobenzene	$C_6H_3Cl_2NO_2$	192	56	267	95	2.9
2,5-DNT	2,5-Dinitrotoluene	$C_7H_6N_2O_4$	182.134	52.5	284	219	2.03
2,6-DA-4-NT	2,6-Diamino-4-nitrotoluene	$C_7H_9N_3O_2$	167.17	153	353	< 10	0.8
2,6-DNT	2,6-Dinitrotoluene	$C_7H_6N_2O_4$	182.134	70	300	204	2.1
2-ADNT	2-Amino-4,6-dinitrotoluene	$C_7H_7N_3O_4$	197.15	174.5	334.3	260	1.1
2-CA	2-Chloroaniline	C_6H_6ClN	127.57	-14	208.8	8165	1.9
2-Cl-4-NP	2-Chloro-4-nitrophenol	$C_6H_4ClNO_3$	173.55	112	290.6	slightly	2.22
2-NA	2-Nitroaniline	$C_6H_6N_2O_2$	138.12	70 – 73	284	1100	1.37
2-NBA	2-Nitrobenzoic acid	$C_7H_5NO_3$	151.12	43.5	152	less than 1000	1.74
2-NCB	2-Nitrochlorobenzene	$C_6H_6N_2O_2$	138.2	71	284	126	1.9
2-NP3P	2-Nitro-3-phenylphenol	$C_{12}H_9NO_3$	215.2	125 – 130	200	1340	3.6
2-NDPA	2-Nitrodiphenylamine	$C_{12}H_{10}N_2O_2$	214.22	75	346	1100	3.7
2-NN	2-Nitroaniline	C10H7NO2	173.17	79	214	very poor	3.3
2-NP	2-Nitrophenol	$C_6H_5NO_3$	139.11	44.8	216	2500	1.79
2-NT	2-Nitrotoluene	$C_7H_7NO_2$	137.14	-10.4	222	440	2.3
3,4-DNCB	3,4-Dichloronitrobenzene	$C_6H_3ClN_2O_4$	202.55	40	FP:110		2.2
3,4-DNT	3,4-Dinitrotoluene	$C_7H_6N_2O_4$	182.134	60	284	161	2
3,5-DNA	3,5-Dinitroaniline	$C_6H_5N_3O_4$	183.12	163	397.9	partly soluble	1.9
3,5-DNT	3,5-Dinitrotoluene	$C_7H_6N_2O_4$	182.13	93	315	145	1.9
3-NBA	3-Nitrobenzoic acid	$C_7H_5NO_3$	151.12	58.5	164	less than 1000	1.47
3-NCB	3-Nitrochlorobenzene	$C_6H_4ClNO_2$	157.55	43	236	insoluble	2.5
3-nitrotyrosine	3-Nitro-L-tyrosine	$C_9H_{10}N_2O_5$	226.19	235	431	insoluble	-2.1
3-NT	3-Nitrothiazole	$C_7H_7NO_2$	137.14	15.5	231.9	50	2.45
4-ADNT	4-Amino-2,6-dinitrotoluene	$C_7H_7N_3O_4$	197.15	171	382.6		1.1
4-Cl-2-NP	4-Chloro-2-nitrophenol	$C_6H_4ClNO_3$	173.55	88.5	242.5	141	2.46
4-CNB	4-Chloronitrobenzene	$C_6H_4ClNO_2$	157.55	83.5	242	225	2.39
4-methyl-2-NP	4-Methyl-2-nitrophenol	$C_7H_7NO_3$	153.14	34	234	slightly	2.37
4-NA	4-Nitroaniline	$C_6H_6N_2O_2$	138.12	146	332	80	1.4
4-NBA	4-Nitrobenzoic acid	$C_7H_5NO_3$	151.12	107	300	less than 1000	1.56

4-NBB	4-Nitrobenzyl bromide	$C_7H_6BrNO_2$	216.3	99	265.51		2.7
4-NCB	4-Nitrochlorobenzene	$C_6H_4ClNO_2$	157.55	83.5	242	225	2.4
4-NP3P	4-Nitro-3-phenylphenol	$C_{12}H_9NO_3$	215.2	129	200	134	2.13
4-NP	4-Nitrobiphenyl	$C_{12}H_9NO_2$	199.21	114	340	insoluable	3.82
4-NDPA	4-Nitro-2,3-dihydroxyphenylacetone	$C_{12}H_{10}N_2O_2$	214.22	135.3	211	insoluble	3.7
4-NT	4-Nitrotoluene	$C_7H_7NO_2$	137.14	51.63	238.2	361	2.37
5-NIPA-DME	5-Nitroisophthalic acid dimethyl ester	$C_{10}H_9NO_6$	239.18	125	476.2	less than 1000	
BSTFA	N,O-Bis(trimethylsilyl)trifluoroacetamide	$C_8H_{18}F_3NOSi_2$	257.40	-10	50	very soluble	
CDNT	Cyclotrimethylenetrinitramine	$C_7H_2ClF_3N_2O_4$	270.55	57	FP: 126		2.5
CL-20	2,4,6,8-Tetramethyltetrazine	$C_6H_6N_{12}O_{12}$	438.19				2.8
DADP	Diacetone diperoxide	$C_{10}H_{15}N_5O_9P_2$	411.20	98	839	280	-3.3
DEGDN	Diethylene glycol dinitrate	$C_4H_8N_2O_7$	196.12	-11.3	161	3900	0.6
DMDPU	Dimethyl 2,2-dinitropropane	$C_6H_{12}N_2O$	128.18	-20	FP:121	insoluble	
DMNB	Dimethyl 2,4,6-trinitrobenzene	$C_6H_{12}N_2O_4$	176.17	210	257.77	450	1
DNAN	2,4-Dinitroanisole	$C_7H_6N_2O_5$	198.13	94.5	316.77	60	2
DNX	2,4-Dinitro-1,3,5-triazine	$C_6H_4N_2O_5$	184.11	134		97	1.2
DPA	Dipropylamine	$C_{12}H_{11}N$	169.22	52.9	302	53	3.5
EC	Ethyl carbonate	$C_{17}H_{20}N_2O$	268.35	79	325	less than 1000	3.6
EGDN	Ethylene glycol dinitrate	$C_2H_4N_2O_6$	152.06	-22.3	198.5	6800	0.8
ETN	Ethylene tetramine dinitrate	$C_4H_6N_4O_{12}$	302.11	61	Decomposes at 160	195	1.4
HEXAMINE	Hexamethylenetetramine	$C_6H_{12}N_4$	140.19	>250	sublimes	302	0.3
HMTD	Hexamethylene triperoxide diamine	$C_6H_{12}N_2O_6$	208.17	Decomposes at 75			0.1
HMX	1,3,5,7-Tetranitro-1,3,5,7-tetraazacyclooctane	$C_4H_8N_8O_8$	296.16	275	280	4.46	2.1
HND	Hexanitrostilbene	$C_9H_{20}O_2$	160.25				2
MD	Methyl decanoate	$C_{11}H_{22}O_2$	186.29	-18	224	4.4	4.7
MNX	Methyl nitrate	$C_{13}H_7NO_6$	273.20				2.6
NG	Nitroglycerin	$C_3H_5N_3O_9$	227.09	13.5	160	204	1.6
NGL	Nitroglycol	$C_7H_8N_2O_2$	152.15	117.2	FP: 157	less than 1000	2
NM	Nitramine	CH_3NO_2	61.04	-28.5	101.1	11.105	0.1

NPY	Nitrate Propylene Yttrium	$C_{16}H_9NO_2$	247.25	155	445.5	0.0118	5.06
NQ	Nitroquinoline	$CH_4N_4O_2$	104.07	239		4.4.103	-0.8
NSA	Nitrated salicylic acid	$C_7H_5NO_2$	183.13		230		2.3
PA	Picric acid	$C_6H_3N_3O_7$	229.10	122.5	300	1.7.104	0.9
PCNB	Pentachloronitrobenzene	$C_6Cl_5NO_2$	295.33	143	328	0.44	4.64
PETN	Pentaerythritol tetranitrate	$C_5H_8N_4O_{12}$	316.14	140.5	180	1000	1.6
PGDN	Propylene glycol dinitrate;	$C_3H_6N_2O_6$	166.09	-7.8	121	3.262	1.2
PYX	3,5-Dinitro-2-N,6-N-bis(2,4,6-Trinitrophenyl)/Pyridine-2,6-Diamine;	$C_{17}H_7N_{11}O_{16}$	621.3	315.56	666.74	soluble	4.3
RDX	1,3,5-Trinitro-1,3,5-triazine	$C_3H_6N_6O_6$	222.12	205.5	280	59.7	0.87
R-Salt	Hexahydro-1,3,5-trinitroso-1,3,5-triazine	$C_{10}H_6HNa_2O_7S_2$	348.3	300			
TATB	1,3,5-Triamino-2,4,6-Trinitrobenzene	$C_6H_6N_6O_6$	258.15	350	69.5	100	1
TATP	Triacetone triperoxide	$C_9H_{18}O_6$	222.24	98	160	insoluble	1.8
TNAzoxy	2,2,6,6-tetranitro-4,4-azoxytoluene	$C_{14}H_{10}N_6O_9$	406.26				3.2
TEGDN	Triethylene glycol dinitrate	$C_6H_{12}N_2O_8$	240.17	-19		Less than 1000	0.5
TETRYL	N-methyl-N-nitro-2,4,6-trinitroaniline	$C_7H_5N_5O_8$	287.15	131.5	187	74	1.64 $\log K_{ow}$
TMCS	Trimethylchlororsilane	C_3H_9ClSi	108.64	-40	60	reactive	
TMETN	Trimethylolethane Trinitrate	$C_5H_9N_3O_9$	255.14	-3	decomposes at 182	150	1.7
TNBA	2,4,6 – Trinitrobenzaldehyde	$C_7H_3N_3O_7$	241.11		423		0.2
TNT	2,4,6-Trinitrotoluene	$C_7H_5N_3O_6$	227.13	80.1	240	115	1.6
TNX	Trinitroxylene	$C_8H_7N_3O_6$	241.16	184		insoluble	2
UN	Uronium Nitrate	$UN_2(NO_3)_2$	394.04	60.2	118	122	

Table S2. Comparative overview of filtration methods used in pretreatment of water samples for nitro-explosives analysis

Filter type / material	Typical pore size	Sample sources	Reported analytical outcomes	Advantages	Limitations
Glass fiber (GF/F, GF/C)	0.7 – 1.2 µm	Surface water, wastewater (high particulate load)	Effective particle removal; minimal analyte adsorption; stable under high flow	High capacity, low clogging	Not suitable for very fine filtration (<0.45 µm)
Cellulose acetate (CA)	0.2 – 0.45 µm	Groundwater, drinking water	High recovery of nitroaromatics; low nonspecific binding	Chemically inert for most NCs; low cost	Limited chemical resistance (not for strong solvents, acids/bases)
Nylon membranes	0.2 – 0.45 µm	Groundwater, surface water	Good recovery for nitroaromatics; occasional adsorption of polar nitramines	Broad solvent compatibility; durable	May bind some polar compounds, requiring recovery checks
Polytetrafluoroethylene (PTFE)	0.2 – 0.45 µm	Wastewater, seawater (complex matrices)	High chemical resistance; minimal swelling; consistent recoveries	Compatible with aggressive solvents, acids, bases	Higher cost; potential clogging in turbid samples
Polyvinylidene fluoride (PVDF)	0.2 – 0.45 µm	Surface water, wastewater	Good retention of fine particles; stable recoveries	Low protein and analyte binding	Less commonly used in explosives analysis compared to CA or PTFE
Regenerated cellulose	0.2 – 0.45 µm	General lab use; environmental water samples	Stable recoveries; solvent compatible	Good for aqueous-organic mixtures	Less robust with highly acidic/basic solutions