

Energetic Crystal Engineering via Intermolecular Interactions: From Fundamental Understanding to Advanced Application

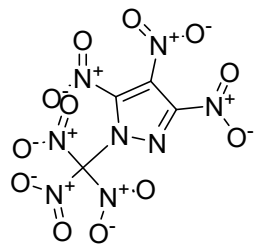
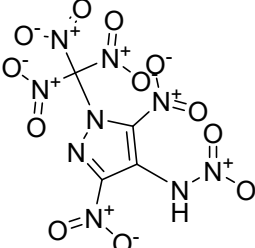
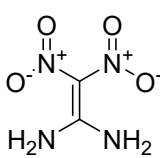
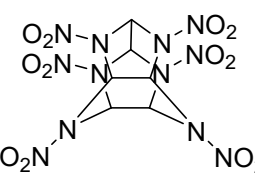
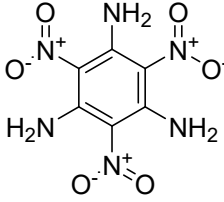
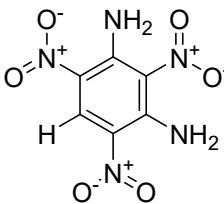
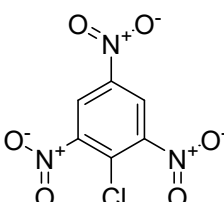
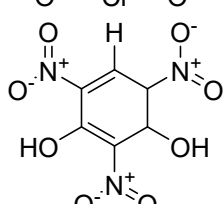
Shiyong Chen ^a, Hui Wang ^b, Yuan Gao ^{*,a}, Xin Huang ^{*,b}, Hongxun Hao ^b

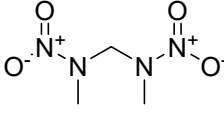
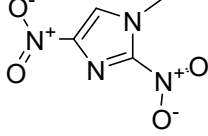
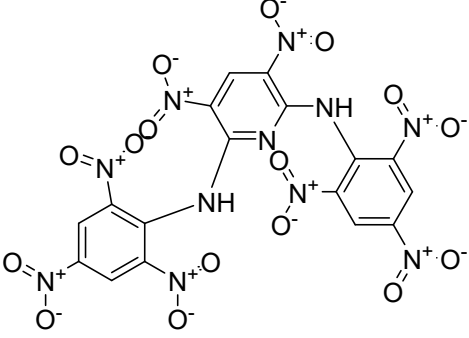
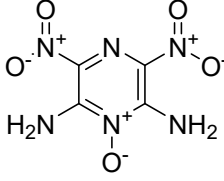
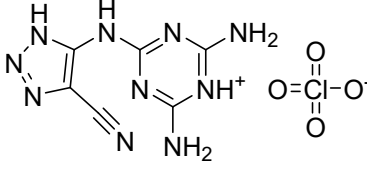
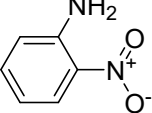
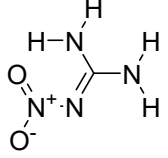
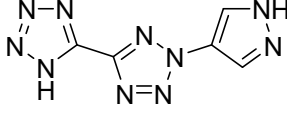
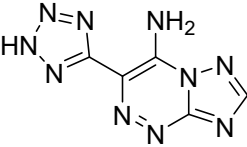
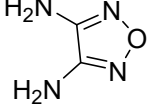
Scheme S1. Molecular structures of the mentioned compounds.

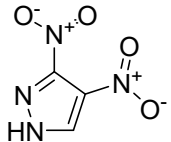
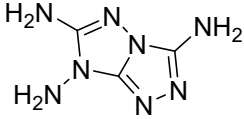
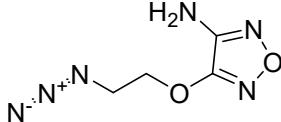
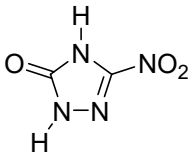
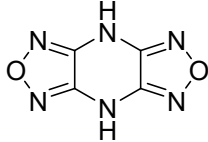
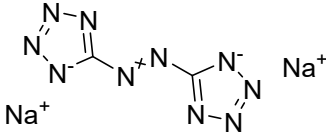
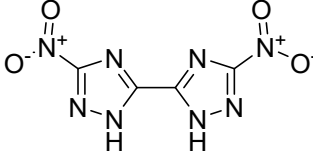
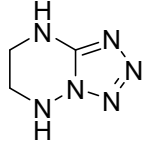
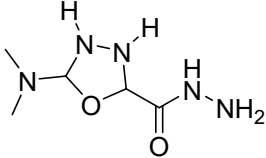
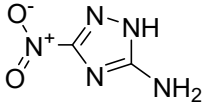
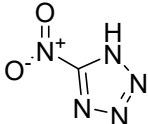
Compound Name	Abbreviation	Molecular Structure
1 <i>H</i> ,1' <i>H</i> -5,5'-Bitetrazole-1,1'-diolate	BTO	
1 <i>H</i> ,4 <i>H</i> -3,6-Dinitropyrazolo[4,3- <i>c</i>]pyrazole	DNPP	
1-Amino-1,2,3-triazole	ATZ	
1-Methyl-3,4,5-trinitropyrazole	MTNP	
1-Methyl-3,5-dinitro-1,2,4-triazole	MDNT	
1-Methyl-4,5-dinitroimidazole	4,5-MDNI	
1-Nitronaphthalene	NNAP	

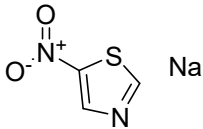
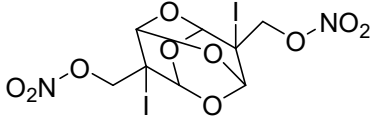
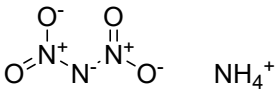
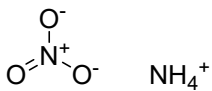
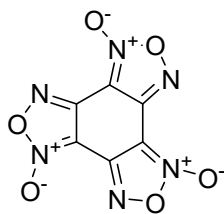
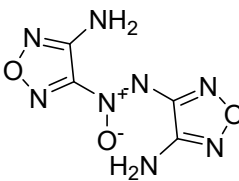
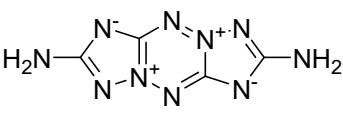
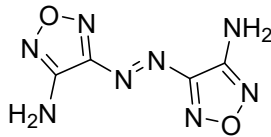
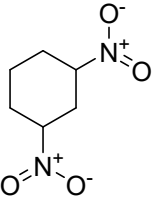
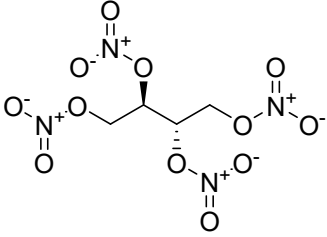
^aSchool of Chemistry and Chemical Engineering, Nanjing University of Science and Technology, Nanjing, 210094, China.

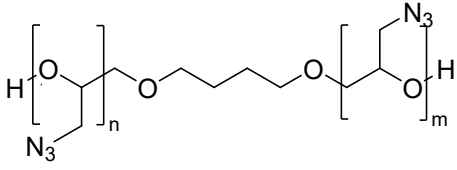
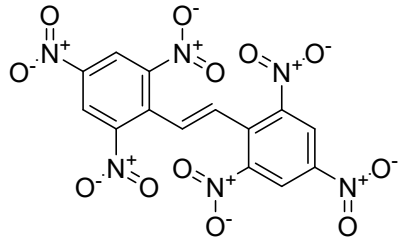
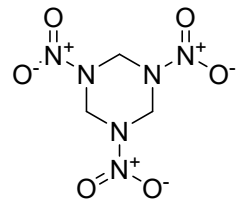
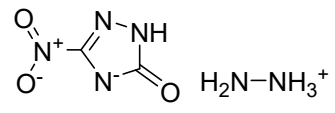
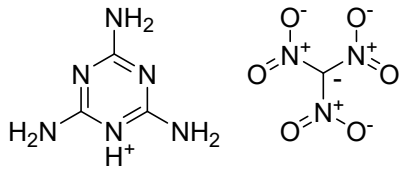
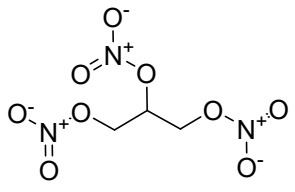
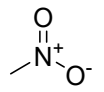
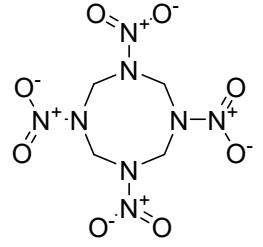
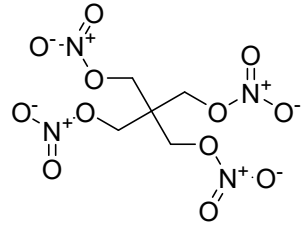
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1-Trinitromethyl-3,4,5-trinitropyrazole	TTP	
1-Trinitromethyl-3,5-dinitro-4-nitroaminopyrazole	DNTP	
2,2-Dinitroethene-1,1-diamine	FOX-7	
2,4,6,8,10,12-Hexanitro-2,4,6,8,10,12-hexaazaisowurtzitane	CL-20	
2,4,6-Trinitrobenzene-1,3,5-triamine	TATB	
2,4,6-Trinitrobenzene-1,3-diamine	DATB	
2,4,6-Trinitrochlorobenzene	TNCB	
2,4,6-Trinitrocyclohexa-1,5-diene-1,3-diol	DNDP	

2,4-Dinitro-2,4-diazapentane	DNDAP	
2,4-Dinitroimidazole	2,4-MDNI	
2,6-Bis(picrylamino)-3,5-dinitropyridine	PYX	
2,6-Diamino-3,5-dinitropyrazine-1-oxide	LLM-105	
2,6-Diamino-4-((5-cyano-1 <i>H</i> -1,2,3-triazol-4-yl)amino)-1,3,5-triazin-1-ium perchlorate	-	
2-Nitroaniline	ONA	
2-Nitroguanidine	NQ	
2'-(1 <i>H</i> -Pyrazol-4-yl)-1 <i>H</i> ,2'- <i>H</i> -5,5'-bistetrazole	-	
3-(2 <i>H</i> -Tetrazol-5-yl)-[1,2,4]triazolo[5,1- <i>c</i>][1,2,4]triazin-4-amine	-	
3,4-Diaminofurazan	DAF	

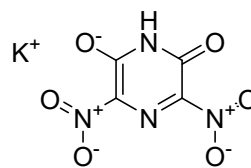
3,4-Dinitropyrazole	3,4-DNP	
3,6,7-Triamino-7 <i>H</i> -[1,2,4]triazolo[4,3- <i>b</i>][1,2,4]triazole	TATOT	
3-Amino-4-azidoethoxyfurazan	AAeF	
3-Nitro-1,2,4-triazol-5-one	NTO	
4 <i>H</i> ,8 <i>H</i> -Bis([1,2,5]oxadiazolo)[3,4- <i>b</i> :3',4'- <i>e</i>]pyrazine	DFP	
5,5'-Azotetrazole sodium	-	
5,5'-Dinitro-2 <i>H</i> ,2 <i>H'</i> -3,3'-bi-1,2,4-triazole	DNBT	
5,6,7,8-Tetrahydrotetrazolo[1,5- <i>b</i>][1,2,4]-triazine	TZTN	
5-Amino-1,3,4-oxadiazole-2-carbohydrazide	HAOC	
5-Amino-3-nitro-1 <i>H</i> -1,2,4-triazole	ANTA	
5-Nitrotetrazole	-	

5-Nitrothiazole sodium	-	
9,10-Bis(nitratomethyl)-9,10-diiido-2,4,6,8-tetraoxadamantane	-	
Ammonium dinitramide	ADN	
Ammonium nitrate	AN	
Benzotrifuroxan	BTF	
Diaminoazoxyfurazan	DAAF	
Diaminobistriazolotetrazine dizwitterion	TYX-1	
Diaminohydrazofurazan	DAAzF	
Dinitrobenzene	DNB	
Erythritol tetranitrate	ETN	

Glycidyl azide polymer	GAP	
Hexanitrostilbene	HNS	
Hexogen	RDX	
Hydrazine 3-nitro-1,2,4-triazol-5-one	HNTO	
Melaminium nitroformate	MaNF	
Nitroglycerin	-	
Nitromethane	-	
Octogen	HMX	
Pentaerythritol tetranitrate	PETN	

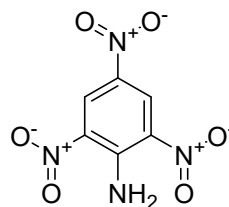
Potassium 3,5-dinitro-6-oxo-1,6-dihydropyrazin-2-olate

KDNODP



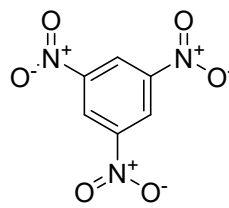
Trinitramide

TNA



Trinitrobenzene

TNB



Trinitrotoluene

TNT

