Crystal Packing of Sensitive High Energetic Explosives

Yu Ma,[†] Anbang Zhang,[†‡] Xianggui Xue,[†] Daojian Jiang,[†] Yuanqiang Zhu,[‡] and Chaoyang Zhang*[†]

[†] *Institute of Chemical Materials, China Academy of Engineering Physics (CAEP), P. O. Box 919-327, Mianyang, Sichuan 621900, China.*
[‡] *College of Chemistry and Chemical Engineering, Southwest Petroleum University, Chengdu, Sichuan 610500, China.*

Supporting Information

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S1. Crystallographic information of 10 SHEs discussed.

Table s1. Crystallographic information of ten SHEs discussed.

Explosives	ONDO[1]	PETN[2]	TNAZ[3]	RDX[4]	β-HMX[5]
Refcode	DILFUZ	PERYTN10	CIWMEA10	CTMTNA	OCHTET12
Formula	$C_6H_8N_{10}O_{16}$	$C_5H_8N_4O_{12}$	$C_3H_4N_4O_6$	$C_3H_6N_6O_6$	$C_4H_8N_8O_8$
Symmetry	Monoclinic	Tetragonal	Orthorhombic	Orthorhombic	Monoclinic
Space group	P21/n(14)	P-42$_1$/c	Pbca	Pbca	P21/c
a(Å)	5.972(<1)	9.38	5.733(1)	13.182(2)	6.540
b(Å)	12.017(1)	9.38	11.127(2)	11.574(2)	11.050
c(Å)	11.841(1)	6.7	21.496(4)	10.709(2)	8.700
α(º)	90	90	90	90	90
β(º)	97.11	90	90	90	124.3
γ(º)	90	90	90	90	90
V(Å^3)	843.156	589.495	1371.253	1633.856	519.387
Z	2	2	8	8	2
Density(g/cm^3)	1.876	1.781	1.861	1.806	1.894
Explosives	BCHMX[6]	BTF[7]	HNB[8]	ε-CL-20[9]	ONC[10]
Refcode	UGUGIM	BZOFOX	HNOBEN	PUBMUU02	CUGDIR
Formula	$C_4H_6N_8O_8$	$C_6N_6O_6$	$C_6N_6O_{12}$	$C_6H_6N_{12}O_{12}$	$C_8N_8O_{16}$
Symmetry	Monoclinic	Orthorhombic	Monoclinic	Monoclinic	Monoclinic
Space group	P21(4)	Pna21	I2/c	P21/n	C2/c
a(Å)	8.598(<1)	6.923(1)	13.220(30)	8.852(2)	12.785(<1)
b(Å)	6.950(<1)	19.516(1)	9.130(40)	12.556(3)	8.840(<1)
c(Å)	8.973(<1)	6.518(1)	9.680(30)	13.386(3)	13.924
α(º)	90.00	90	90	90	90
β(º)	101.78(<1)	90	95.5	106.82	98.03
γ(º)	90.00	90	90	90	90
V(Å^3)	524.826	880.642	1162.984	1424.146	1558.173
Z	2	4	4	4	4
Density(g/cm^3)	1.861	1.901	1.988	2.044	1.978

S2. Intramolecular hydrogen bonds in ONDO.

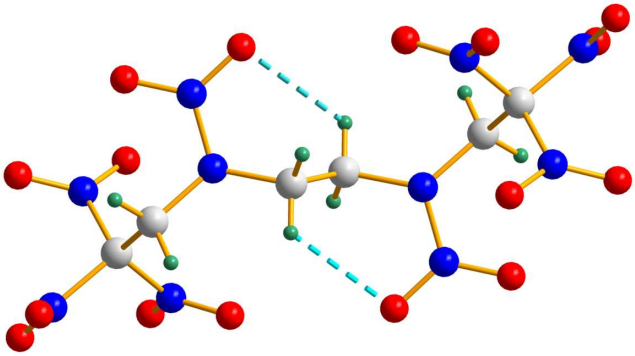

Figure s1. Intramolecular hydrogen bonds in ONDO denoted by dash.

Table s2. Geometry and AIM analyses of the intramolecular HBs in related molecules.

Molecule	D-H, Å	H···A, Å	A···D, Å	A-H···D,°	ρ, e/Å^3	*v*, a.u.	E_{HB}, kJ/mol	ΣE_{HB}, kJ/mol
ONDO	0.907	2.533	2.999	112.5	0.0058	-0.0039	5.1	10.2

S3. References.

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