Supporting Information for

Communication

Convenient Preparation, Thermal Properties and X-ray Structure Determination of 2,3-Dihydro-5,6,7,8-tetranitro-1,4-benzodioxine (TNBD): A Promising High-Energy-Density Material

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Table S1: X-ray difraction analysis data. Geometry tables for the compound TNBD.

INTRAMOLECULAR BOND LENGTHS

Minimum bond length= 0.80Å : Maximum bond length= 1.60Å

O(1)	C(9)	1.338(2)	O(1)	C(2)	1.453(2)
O(82)	N(8)	1.212(2)	O(72)	N(7)	1.212(2)
O(81)	N(8)	1.225(2)	N(7)	O(71)	1.215(2)
N(7)	C(7)	1.473(2)	N(8)	C(8)	1.472(2)
C(7)	C(7)	1.383(3)	C(7)	C(8)	1.388(2)
C(9)	C(9)	1.405(3)	C(9)	C(8)	1.391(2)
C(2)	C(2)	1.503(3)	C(2)	H(2A)	0.92(3)
C(2)	H(2B)	0.91(2)			

INTRAMOLECULAR BOND ANGLES

Minimum bond length= 0.80Å : Maximum bond length= 1.60Å

C(9) - O(1) - C(2)	113.81(11)	O(72) - N(7) - O(71)	126.22(14)
O(72) - N(7) - C(7)	116.99(12)	O(71) - N(7) - C(7)	116.79(12)
O(82) - N(8) - O(81)	126.22(13)	O(82) - N(8) - C(8)	117.17(12)
O(81) - N(8) - C(8)	116.61(13)	N(7) - C(7) - C(7)	121.79(8)

N(7) - C(7) - C(8) 118.94(13) C(7) - C(7) - C(8) 119.18(8)
O(1) - C(9) - C(9) 122.69(7) O(1) - C(9) - C(8) 118.69(12)
C(9) - C(9) - C(8) 118.60(8) N(8) - C(8) - C(7) 120.19(12)
N(8) - C(8) - C(9) 117.51(12) C(7) - C(8) - C(9) 122.21(14)
O(1) - C(2) - C(2) 110.23(11) O(1) - C(2) - H(2A) 108.(2)
O(1) - C(2) - H(2B) 105.6(15) C(2) - C(2) - H(2A) 106.(2)
C(2) - C(2) - H(2B) 111.9(14) H(2A) - C(2) - H(2B) 115.(2)

INTRAMOLECULAR TORSION ANGLES (H omitted)

Minimum bond length= 0.80Å : Maximum bond length= 1.60Å

C(2) - O(1) - C(9) - C(9) 167.41(11) C(2) - O(1) - C(9) - C(8) 165.99(13)
C(9) - O(1) - C(2) - C(2) -136.50(10) O(72) - N(7) - C(7) - C(7) 43.76(9)
O(72) - N(7) - C(7) - C(8) 47.05(10) O(71) - N(7) - C(7) - C(7) -135.42(12)
O(71) - N(7) - C(7) - C(8) -132.12(14) O(82) - N(8) - C(8) - C(7) -113.15(13)
O(82) - N(8) - C(8) - C(9) 70.38(11) O(81) - N(8) - C(8) - C(7) 67.25(11)
O(81) - N(8) - C(8) - C(9) -109.22(12) C(7) - C(7) - N(7) - O(72) -136.24(14)
N(7) - C(7) - C(7) - N(7) 0.00(8) C(7) - C(7) - N(7) - O(71) 44.58(11)
N(7) - C(7) - C(7) - C(8) -176.70(13) C(8) - C(7) - N(7) - O(72) 47.05(10)
C(8) - C(7) - N(7) - O(71) -132.12(14) N(7) - C(7) - C(8) - N(8) 0.40(9)
N(7) - C(7) - C(8) - C(9) 176.7(2) C(8) - C(7) - C(7) - N(7) 176.70(12)
C(7) - C(7) - C(8) - N(8) -176.39(15) C(7) - C(7) - C(8) - C(9) -0.09(10)

C(8) - C(7) - C(7) - C(8) 0.00(8) O(1) - C(9) - C(9) - O(1) 0.00(7)

O(1) - C(9) - C(9) - C(8) 178.59(13) C(9) - C(9) - O(1) - C(2) -12.59(9)

O(1) - C(9) - C(8) - N(8) -1.20(8) O(1) - C(9) - C(8) - C(7) -177.6(2)

C(8) - C(9) - O(1) - C(2) 165.99(13) C(8) - C(9) - C(9) - O(1) -178.59(12)

C(9) - C(9) - C(8) - N(8) 177.44(14) C(9) - C(9) - C(8) - C(7) 1.05(10)

C(8) - C(9) - C(9) - C(8) 0.00(8) C(7) - C(8) - N(8) - O(82) -113.15(13)

C(7) - C(8) - N(8) - O(81) 67.25(11) N(8) - C(8) - C(7) - N(7) 0.40(9)

N(8) - C(8) - C(7) - C(7) 3.61(8) N(8) - C(8) - C(9) - O(1) -1.20(8)

C(9) - C(8) - N(8) - O(82) 70.38(11) C(9) - C(8) - N(8) - O(81) -109.22(12)

N(8) - C(8) - C(9) - C(9) -2.56(7) C(7) - C(8) - C(9) - O(1) -177.6(2)

C(9) - C(8) - C(7) - N(7) 176.7(2) C(9) - C(8) - C(7) - C(7) 179.90(13)

C(7) - C(8) - C(9) - C(9) -178.95(13) O(1) - C(2) - C(2) - O(1) -0.02(7)

C(2) - C(2) - O(1) - C(9) 43.50(10)

INTERMOLECULAR NON-BONDED DISTANCES

Minimum distance= 1.95Å : Maximum distance= 3.50Å

Atom(1)	Atom(2)	distance	ns	np	Ta	Tb	Tc	x(2)	y(2)	z(2)
O(1)	O(82)	3.0534(15)	3	1	0	0	1	0.19772	0.08779	0.59972
O(1)	O(71)	3.235(2)	2	1	0	1	1	-0.03531	0.22086	0.61436
O(1)	N(8)	3.448(2)	3	1	0	0	1	0.29370	0.04775	0.56425
O(82)	H(2A)	3.03(3)	3	1	0	0	1	0.42330	0.46537	0.67214
O(82)	H(2B)	3.25(2)	3	1	0	0	1	0.53069	0.38884	0.62140
O(72)	O(81)	3.388(2)	3	1	0	1	1	0.31223	1.00975	0.45335

O(72) - C(7)	3.457(2)	5	1	0	0	0	-0.05135	0.57427 0.20630
O(81) - C(7)	3.262(2)	2	1	0	1	1	-0.05135	0.42573 0.70630
O(81) - C(8)	3.220(2)	6	1	0	1	0	0.10141	0.54512 0.83681
O(81) - C(2)	3.461(2)	3	1	0	0	1	0.47263	0.39265 0.68007

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ns is the symmetry operator number - (* denotes inversion indicator)
np is the lattice point number

DIHEDRAL ANGLES FORMED BY LSQ PLANES

PLANE - PLANE	ANGLE	E.S.D
PLANE 1 (C5 C6 C7 C8 C9 C10); PLANE 2 (O71 N7 O72); PLANE 3 (O81 N8 O82)		
1 2	46.143	0.081
1 3	68.706	0.103