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Research paper

1,3,6,8-Tetranitrocarbazole (TNC): Efficient One-Pot Synthesis, X-ray Crystallographic Analysis, and Property Evaluation

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1,3,6,8-Tetranitrocarbazole (TNC) crystal H-bonds description

A wide net of the hydrogen bonding is a characteristic feature of the TNC crystal structure:

Centric cell of lattice type P symmetry operations

1) $-X, 1/2+Y, 1/2-Z$

2) $X, 1/2-Y, 1/2+Z$

3) X, Y, Z

4) $-X, -Y, -Z$

Atoms from identity symmetry acting as donors:

Hydrogen Bridge D...A(A) D-H(A) H...A(A) D-H...A(Degr..)

1) N9 - H9 ... O15

(555 1) (555 1) (555 1) 2.719(3) 0.87(3) 2.26(3) 113(2)

2) N9 - H9 ... O25

(555 1) (555 1) (555 1) 2.728(3) 0.87(3) 2.25(3) 115(2)

3) C4 - H4 ... O21

(555 1) (555 1) (455 4) 3.341(3) 0.95 2.43 160

4) C7 - H7 ... O15

(555 1) (555 1) (454 2) 3.375(3) 0.96 2.50 151

Table S1. TNC bond lengths

Bond	Bond length [Å]	Bond	Bond length [Å]
N(20)-O(22)	1.220(3)	N(23)-C(8)	1.458(3)
N(20)-O(21)	1.235(3)	N(14)-O(16)	1.216(3)
N(20)-C(6)	1.463(3)	N(14)-C(1)	1.456(3)
C(5)-C(6)	1.383(3)	C(8)-C(7)	1.372(4)
C(5)-C(12)	1.385(3)	C(8)-C(13)	1.393(3)
C(5)-H(5)	1.03	C(6)-C(7)	1.391(3)
O(15)-N(14)	1.236(3)	C(3)-C(2)	1.386(4)
C(12)-C(13)	1.419(3)	C(3)-C(4)	1.385(3)
C(12)-C(11)	1.444(3)	C(3)-N(17)	1.461(4)
C(11)-C(4)	1.382(3)	C(4)-H(4)	0.95
C(11)-C(10)	1.416(3)	C(2)-C(1)	1.378(4)
N(9)-C(13)	1.373(3)	C(2)-H(2)	1.01
N(9)-C(10)	1.370(3)	C(7)-H(7)	0.96
N(9)-H(9)	0.87(3)	C(1)-C(10)	1.395(3)
N(23)-O(24)	1.213(3)	N(17)-O(18)	1.211(3)
N(23)-O(25)	1.230(3)	N(17)-O(19)	1.216(3)

Table S2. Selected angles (°) in the TNC molecule

Angle	[°]	Angle	[°]
O(22)-N(20)-O(21)	123.4(2)	C(8)-C(13)-C(12)	119.5(2)
O(22)-N(20)-C(6)	118.8(2)	C(5)-C(6)-C(7)	123.2(2)
O(21)-N(20)-C(6)	117.8(2)	C(5)-C(6)-N(20)	118.6(2)
C(6)-C(5)-C(12)	117.5(2)	C(7)-C(6)-N(20)	118.2(2)
C(6)-C(5)-H(5)	116.92(14)	C(2)-C(3)-C(4)	123.6(2)
C(12)-C(5)-H(5)	125.57(13)	C(2)-C(3)-N(17)	118.1(2)
C(5)-C(12)-C(13)	120.6(2)	C(4)-C(3)-N(17)	118.2(2)
C(5)-C(12)-C(11)	133.3(2)	C(11)-C(4)-C(3)	117.3(2)
C(13)-C(12)-C(11)	106.1(2)	C(11)-C(4)-H(4)	123.74(14)
C(4)-C(11)-C(10)	120.7(2)	C(3)-C(4)-H(4)	118.5(2)
C(4)-C(11)-C(12)	132.6(2)	C(1)-C(2)-C(3)	118.6(2)
C(10)-C(11)-C(12)	106.7(2)	C(1)-C(2)-H(2)	114.2(2)
C(13)-N(9)-C(10)	109.8(2)	C(3)-C(2)-H(2)	126.39(14)
C(13)-N(9)-H(9)	125(2)	C(8)-C(7)-C(6)	118.8(2)
C(10)-N(9)-H(9)	125(2)	C(8)-C(7)-H(7)	120.00(14)
O(24)-N(23)-O(25)	124.1(2)	C(6)-C(7)-H(7)	121.18(14)
O(24)-N(23)-C(8)	118.1(2)	C(2)-C(1)-C(10)	120.1(2)
O(25)-N(23)-C(8)	117.8(2)	C(2)-C(1)-N(14)	119.1(2)
O(16)-N(14)-O(15)	123.9(2)	C(10)-C(1)-N(14)	120.7(2)
O(16)-N(14)-C(1)	118.8(2)	(9)-C(10)-C(1)	131.7(2)
O(15)-N(14)-C(1)	117.3(2)	N(9)-C(10)-C(11)	108.6(2)
C(7)-C(8)-C(13)	120.3(2)	C(1)-C(10)-C(11)	119.7(2)
C(7)-C(8)-N(23)	119.1(2)	O(18)-N(17)-O(19)	124.2(3)
C(13)-C(8)-N(23)	120.5(2)	O(18)-N(17)-C(3)	118.0(2)
N(9)-C(13)-C(8)	131.6(2)	O(19)-N(17)-C(3)	117.9(2)
N(9)-C(13)-C(12)	108.8(2)		

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