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New Journal of Chemistry

Exploring the Reactive Chemistry of FOX-7: Synthesis of Cyclic Triazinane-Based Energetic Materials Featuring FOX-7 Backbone

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Supporting Information

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Table S1. X-ray data and parameters of **1**, **2**, **2·H$_2$O**, **3** and **5.**

	1	**2**	**2·H$_2$O**	**3**	**5**
Chemical formula	$C_5H_5N_7O_8$	$C_9H_{14}N_{10}O_8$	$C_9H_{16}N_{10}O_9$	$C_6H_8N_8O_{10}$	$C_{12}H_{21}ClN_9O_{8.13}$
Formula mass	291.16	390.30	408.32	352.20	456.83
Crystal system	orthorhombic	orthorhombic	monoclinic	monoclinic	monoclinic
a/Å	11.757(3)	16.894(4)	17.038(4)	13.475(6)	13.790(2)
b/Å	12.706(3)	9.096(2)	7.1500(16)	8.538(4)	7.0973(11)
c/Å	13.594(3)	9.676(4)	13.854(3)	13.241(6)	19.700(3)
α/°	90	90	90	90	90
β/°	90	90	99.084(6)	115.838(11)	98.238(4)
γ/°	90	90	90	90	90
Volume/Å^3	2030.8(8)	1486.9(8)	1666.6(7)	1371.1(11)	1908.2(5)
Temperature/K	173	173	173	173	173
Space group	*P*bca	*P*ccn	$P2_1/c$	$P2_1/c$	$P2_1/n$
Z	8	4	4	4	4
Radiation type	Mo-Ka	Mo-Ka	Mo-Ka	Mo-Ka	Mo-Ka
μ/mm^{-1}	0.180	0.153	0.145	0.162	0.267
Density$_{calcd}$/g cm^{-3}	1.905	1.743	1.627	1.706	1.588
F(000)	1184.0	808.0	848.0	720.0	946.0
2Θ range for data collection/°	5.592 to 54.83	4.8 to 50.2	2.4 to 52.8	3.358 to 55.198	3.80 to 54.8
Index ranges	-15/15;-15/15; -17/17	-20/19;-10/10; -11/10	-21/21; -8/8; -17/17	-17/15;-11/11; -16/17	-17/15; -9/9; -25/25
Reflections collected	11814	5877	11113	12162	16374
Independent reflections	2285	1329	3399	3142	4304
R_{int}	0.0788	0.192	0.089	0.1203	0.085
Data/restraints/ parameters	2285/0/181	1329/120/133	3399/0/260	3142/0/217	4304/9/311
R_1 / wR_2 [all data]	0.0818/0.1246	0.1738/0.0735	0.1386/0.1949	0.1813/0.1879	0.1234/0.1716
R_1 / wR_2 [I > 2σ(I)]	0.0496/0.1081	0.0618/0.0735	0.0563/0.1541	0.0676/0.1449	0.0606/0.1666
Goodness-of-fit on F^2	1.040	1.01	1.01	1.001	1.02
CCDC number	1891351	1892967	1892962	1892968	1892969

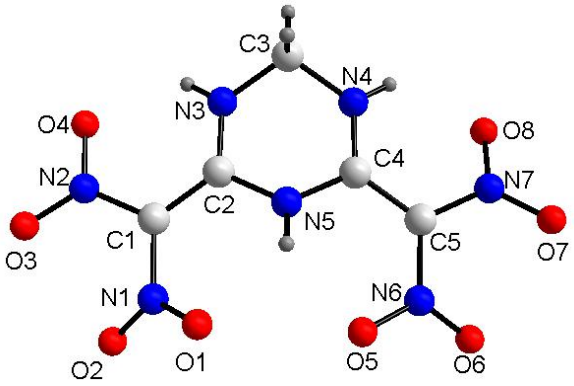


Figure S1. The crystal structure of compound **1**.

Table S2. The bonds length of compound **1**

Parameter	Bond length (Å)	Parameter	Bond length (Å)
O5-N6	1.244(2)	N4-C3	1.458(3)
O6-N6	1.225(2)	N7-C5	1.422(3)
O8-N7	1.240(3)	N3-C2	1.312(3)
O7-N7	1.227(3)	N3-C3	1.451(3)
O1-N1	1.242(3)	O2-N1	1.224(3)
N5-C4	1.373(3)	O4-N2	1.248(3)
N5-C2	1.374(3)	N1-C1	1.432(3)
N6-C5	1.419(3)	N2-C1	1.409(3)
O3-N2	1.234(3)	C4-C5	1.423(3)
N4-C4	1.309(3)	C2-C1	1.412(3)

Table S3. The bonds angles of compound **1**

Parameter	Bond angle (°)	Parameter	Bond length (Å)
C4-N5-C2	122.14(19)	O4-N2-C1	117.8(2)
O5-N6-C5	118.17(19)	N5-C4-C5	120.07(19)
O6-N6-O5	121.4 (2)	N4-C4-N5	115.8(2)
O6-N6-C5	120.45(19)	N4-C4-C5	124.1(2)
C4-N4-C3	118.17(19)	N5-C2-C1	119.4(2)
O8-N7-C5	117.8(2)	N3-C2-N5	115.2(2)
O7-N7-O8	121.9(2)	N3-C2-C1	125.3(2)
O7-N7-C5	120.3(2)	N6-C5-N7	116.71(19)
C2-N3-C3	118.5(2)	N6-C5-C4	112.9(2)
O1-N1-C1	118.4(2)	N7-C5-C4	120.3(2)
O2-N1-O1	122.4(2)	N2-C1-N1	116.0(2)

O2-N1-C1	119.2(2)	N2-C1-C2	121.2(2)
O3-N2-O4	121.7(2)	C2-C1-N1	122.1(2)
O3-N2-C1	120.5(2)	N3-C3-N4	107.8(18)

Table S4. The torsion angles of compound **1**

Parameter	Torsion angle (°)	Parameter	Torsion angle (°)
O1-N1-C1-N2	-142.7(2)	C4-N5-C2-N3	-24.0(3)
O1-N1-C1-C2	28.0(3)	C4-N5-C2-C1	153.4(2)
O2-N1-C1-N2	37.7(3)	C2-N5-C4-N4	25.3(3)
O2-N1-C1-C2	-151.6(2)	C2-N5-C4-C5	-154.5(2)
O3-N2-C1-N1	5.6(3)	O5-N6-C5-N7	167.3(2)
O3-N2-C1-C2	-165.2(2)	O5-N6-C5-C4	-15.9(3)
O3-N2-C1-C2	-175.9(2)	O6-N6-C5-N7	-14.3(3)
O4-N2-C1-C2	13.3(3)	O6-N6-C5-C4	162.5(2)
C3-N3-C2-N5	-14.6(3)	O7-N7-C5-N6	-26.7(3)
C3-N3-C2-C1	168.3(2)	O7-N7-C5-C4	156.4(2)
C2-N3-C3-N4	46.4(3)	O8-N7-C5-N6	154.1(2)
C4-N4-C3-C3	-44.8(3)	O8-N7-C5-C4	-22.9(3)
C3-N4-C4-N5	12.0(3)	N1-C1-C2-N3	179.2(2)
C3-N4-C4-C5	-168.2(2)	N1-C1-C2-N5	2.1(3)
N2-C1-C2-N3	-10.6(4)	N4-C4-C5-N7	5.2(3)
N2-C1-C2-N5	172.3(2)	N5-C4-C5-N6	8.3(3)
N4-C4-C5-N6	-171.5(2)	N5-C4-C5-N7	-174.99(19)

Table S5. The hydrogen bonds in compound **1**

D-H···A	D-H(Å)	H···A(Å)	D···A(Å)	D-H···A(o)
N3—H3···O4	0.8800	2.0100	2.584(3)	122
N3—H3···O8	0.8800	2.3200	3.092(3)	147
N4—H4···O8	0.8800	1.9800	2.590(3)	126
N4—H4···O5	0.8800	2.2500	2.893(3)	130
N5—H5···O1	0.8800	1.9900	2.621(3)	127
N5—H5···O5	0.8800	2.0000	2.560(3)	121
N5—H5···O3	0.8800	2.4400	3.000(3)	122
C3—H3B···O3	0.9900	2.5100	3.280(3)	135
C3—H3B···O7	0.9900	2.4800	3.329(3)	143
C3—H3B···O5	0.9900	2.4900	3.119(3)	121

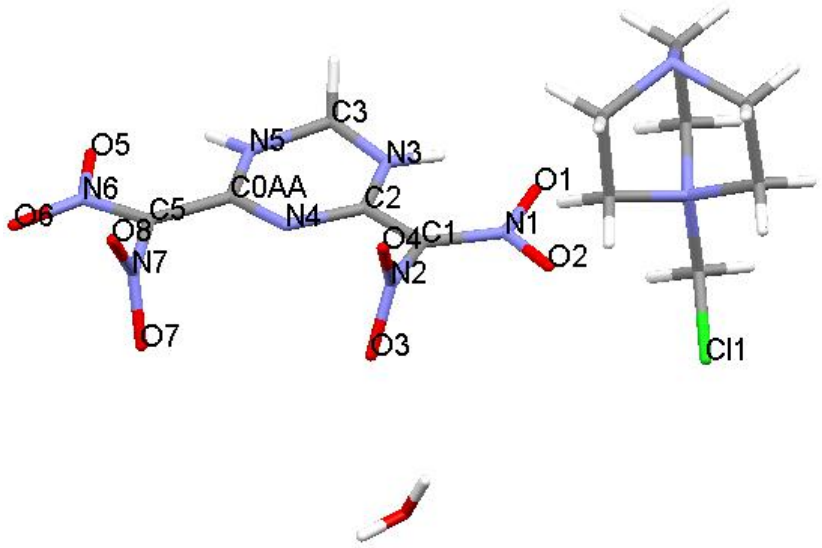


Figure S2. The crystal structure of organic salt **5**.

Table S6. The bonds length of anion in organic salt **5**

Parameter	Bond length (Å)	Parameter	Bond length (Å)
O6-N6	1.259(3)	N4-C0AA	1.335(4)
N7-O8	1.216(4)	N4-C2	1.347(4)
N7-O7	1.213(4)	C0AA-C5	1.411(4)
N7-C5	1.456(4)	N1-O2	1.243(4)
N6-O5	1.250(3)	N1-O1	1.256(5)
N6-C5	1.346(4)	N1-C1	1.365(5)
N5-C0AA	1.309(4)	C2-C1	1.402(5)
N5-C3	1.441(4)	N2-C1	1.44(3)
N3-C2	1.308(4)	N2-O4	1.24(4)
N3-C3	1.428(5)	N2-O3	1.23(5)

Table S7. The bonds angles of anion in organic salt **5**

Parameter	Bond angle (°)	Parameter	Bond length (Å)
O8-N7-C5	118.1(3)	C0AA-C5-N7	118.3(3)
O7-N7-O8	124.1(3)	O2-N1-O1	122.0(4)
O7-N7-C5	117.9(3)	O2-N1-C1	119.5(4)
O6-N6-C5	119.5(2)	O1-N1-C1	118.4(3)
O5-N6-O6	121.1(3)	N3-C2-N4	122.5(3)
O5-N6-C5	119.4(3)	N3-C2-C1	121.7(3)
C0AA-N5-C3	123.3(3)	N4-C2-C1	115.8(3)

C2-N3-C3	124.4(3)	O4-N2-C1	123(3)
C0AA-N4-C2	116.4(3)	O3-N2-C1	117(3)
N5-C0AA-N4	123.5(3)	O3-N2-O4	121(3)
N5-C0AA-C5	121.1(3)	N1-C1-C2	126.9(3)
N4-C0AA-C5	115.4(3)	N1-C1-N2	115.5(11)
N6-C5-N7	114.5(3)	C2-C1-N2	117.1(11)
N6-C5-C0AA	127.3(3)	N3-C3-N5	109.1(3)

Table S8. The torsion angles of anion in organic salt **5**

Parameter	Torsion angle (°)	Parameter	Torsion angle (°)
O1-N1-C1-N2	172.4(12)	C3-N5-C0AA-C5	176.5(3)
O1-N1-C1-C2	-1.4(5)	O5-N6-C5-C0AA	0.9(5)
O2-N1-C1-N2	-7.0(13)	O6-N6-C5-N7	-0.6(4)
O2-N1-C1-C2	179.2(3)	O6-N6-C5-C0AA	179.2(3)
O3-N2-C1-C2	93(2)	O5-N6-C5-N7	-179.0(3)
O4-N2-C1-N1	100(2)	O7-N7-C5-N6	96.1(3)
O3-N2-C1-N1	-82(2)	O7-N7-C5-C0AA	-83.8(4)
O4-N2-C1-C2	-86(2)	O8-N7-C5-N6	-84.3(4)
C3-N3-C2-N4	3.6(5)	O8-N7-C5-C0AA	95.9(3)
C3-N3-C2-C1	-175.9(3)	N1-C1-C2-N3	1.0(5)
C2-N3-C3-N5	-9.7(5)	N1-C1-C2-N4	-178.6(3)
C2-N4-C0AA-N5	-4.3(5)	N2-C1-C2-N3	-172.5(13)
C2-N4-C0AA-C5	176.2(3)	N2-C1-C2-N4	7.9(13)
C0AA-N4-C2-C1	-176.4(3)	N4-C0AA-C5-N6	179.1(3)
C0AA-N4-C2-N3	4.1(5)	N4-C0AA-C5-N7	-1.1(4)
C0AA-N5-C3-N3	9.4(4)	N5-C0AA-C5-N6	-0.4(5)
C3-N5-C0AA-N4	-3.0(5)	N5-C0AA-C5-N7	179.4(3)

Table S9. The bonds length in **2**·H_2O

Parameter	Bond length (Å)	Parameter	Bond length (Å)
O1-N1	1.241(4)	N6-C7	1.448(4)
O4-N2	1.266(4)	N6-C6	1.452(5)
O2-N1	1.252(4)	N6-C5	1.471(5)
O8-N10	1.247(4)	N9-C9	1.390(4)
O5-N9	1.248(4)	N2-O3	1.228(4)
N1-C1	1.382(5)	N2-C1	1.375(5)

N8-C8	1.316(4)	N5-C3	1.444(5)
N8-C6	1.458(5)	N5-C5	1.463(5)
N4-C2	1.323(4)	N5-C4	1.440(5)
N4-C4	1.473(5)	N10-C9	1.366(5)
O7-N10	1.253(4)	N3-C2	1.302(4)
N7-C8	1.310(4)	N3-C3	1.474(5)
N7-C7	1.474(4)	C2-C1	1.467(5)
O6-N9	1.232(4)	C8-C9	1.458(5)

Table S10. The bonds angles in **2·H_2O**

Parameter	Bond angle (°)	Parameter	Bond length (Å)
O1-N1-O2	122.3(3)	O7-N10-C9	123.5(3)
O1-N1-C1	122.0(3)	C2-N3-C3	121.7(3)
O2-N1-C1	115.6(3)	N4-C2-C1	119.3(3)
C8-N8-C6	121.9 (3)	N3-C2-N4	121.0(3)
C2-N4-C4	120.3(3)	N3-C2-C1	119.7(3)
C8-N7-C7	120.9(3)	N8-C8-C9	118.8(3)
C7-N6-C5	114.0(3)	N7-C8-N8	120.6(3)
C6-N6-C7	109.4(3)	N7-C8-C9	120.7(3)
C6-N6-C5	112.0(3)	N1-C1-C2	118.7(3)
O5-N9-C9	115.0(3)	N2-C1-N1	123.9(3)
O6-N9-O5	122.6(3)	N2-C1-C2	117.3(3)
O6-N9-C9	122.4(3)	N9-C9-C8	117.5(3)
O4-N2-C1	114.9(3)	N10-C9-N9	123.5(3)
O3-N2-O4	121.2(3)	N10-C9-C8	117.0(3)
O3-N2-C1	123.9(3)	N6-C7-N7	111.0(2)
C3-N5-C5	114.4(3)	N6-C6-N8	110.3(3)
C4-N5-C3	110.0(3)	N5-C3-N3	110.5(3)
C4-N5-C5	113.7(3)	N6-C5-N5	107.5(3)
O8-N10-O7	120.5(3)	N5-C4-N4	110.8(3)
O8-N10-C9	115.9(3)		

Table S11. The torsion angles in **2·H_2O**

Parameter	Torsion angle (°)	Parameter	Torsion angle (°)
O1-N1-C1-N2	-2.6(4)	C4-N5-C3-N3	-53.2(4)
O1-N1-C1-C2	-178.3(3)	C5-N5-C3-N3	76.2(4)

O2-N1-C1-N2	178.8(3)	C3-N5-C4-N4	54.9(4)
O2-N1-C1-C2	3.2(4)	C5-N5-C4-N4	-74.9(4)
O3-N2-C1-N1	1.4(5)	C3-N5-C5-N6	153.1(3)
O3-N2-C1-C2	177.1(3)	C4-N5-C5-N6	-79.4(3)
O4-N2-C1-N1	179.6(3)	C6-N6-C5-N5	-76.4(3)
O4-N2-C1-C2	-4.7(4)	C7-N6-C5-N5	158.7(3)
C3-N3-C2-N4	1.9(5)	C5-N6-C6-N8	-72.9(4)
C3-N3-C2-C1	-179.1(3)	C7-N6-C6-N8	54.5(4)
C2-N3-C3-N5	25.5(5)	C5-N6-C7-N7	72.5(4)
C4-N4-C2-N3	-0.2(5)	C6-N6-C7-N7	-53.8(4)
C4-N4-C2-C1	-179.3(3)	C8-N7-C7-N6	26.9(4)
C2-N4-C4-N5	-28.8(4)	C7-N7-C8-N8	0.7(5)
C7-N7-C8-C9	-178.6(3)	O8-N10-C9-N9	170.3(3)
C8-N8-C6-N6	-28.9(4)	O8-N10-C9-C8	6.9(4)
C6-N8-C8-N7	0.5(5)	N1-C1-C2-N3	79.8(4)
C6-N8-C8-C9	179.8(3)	N1-C1-C2-N4	-101.1(4)
O5-N9-C9-N10	-171.2(3)	N2-C1-C2-N3	-96.1(4)
O5-N9-C9-C8	-7.9(4)	N2-C1-C2-N4	83.0(4)
O6-N9-C9-N10	9.4(5)	N7-C8-C9-N9	96.2(4)
O6-N9-C9-C8	172.7(3)	N7-C8-C9-N10	-99.3(4)
O7-N10-C9-N9	-11.2(5)	N8-C8-C9-N9	-83.1(4)
O7-N10-C9-C8	-174.6(3)	N8-C8-C9-N10	81.4(4)

Table S12. The hydrogen bonds in **2**·H_2O

D-H···A	D-H(Å)	H···A(Å)	D···A(Å)	D-H···A(o)
N3—H3···O1	0.8800	2.5500	2.916(4)	106.00
N3—H3···O4	0.8800	2.0600	2.897(4)	159.00
N4—H4···O2	0.8800	2.4900	3.110(4)	128.00
N4—H4···O4	0.8800	2.3900	3.103(4)	138.00
N7—H7···O9	0.8800	1.9400	2.788(4)	160.00
N8—H8···O6	0.8800	2.5600	3.248(4)	135.00
N8—H8···O7	0.8800	2.0100	2.829(4)	153.00
O9—H9A···O7	0.8700	2.5300	3.211(4)	136.00
O9—H9B···N6	0.7700	2.2200	2.969(4)	164.00
C3—H3A···O9	0.9900	2.4700	3.444(5)	166.00

C5—H5A···O1	0.9900	2.5100	3.327(5)	139.00
C5—H5B···N8	0.9900	2.6200	2.988(5)	102.00
C6—H6A···O8	0.9900	2.2400	3.209(5)	167.00
C6—H6B···O6	0.9900	2.4600	3.426(5)	165.00
C6—H6B···N5	0.9900	2.6200	2.984(5)	102.00
C7—H7A···O1	0.9900	2.4700	3.338(6)	146.00
C7—H7A···O3	0.9900	2.4300	3.317(5)	148.00
C7—H7B···O6	0.9900	2.4800	3.472(4)	176.00

Table S13. The bonds length in **2**

Parameter	Bond length (Å)	Parameter	Bond length (Å)
O4-N5	1.258(4)	N1-C4	1.424(4)
N3-C3	1.330(5)	N2-C3	1.309(5)
N3-C4	1.464(5)	N2-C2	1.471(5)
N5-O3	1.227(5)	N4-C5	1.414(5)
N5-C5	1.402(5)	N4-O2	1.341(13)
O1-N4	1.220(5)	N4-O2A	1.183(12)
N1-C1	1.472(5)	C3-C5	1.453(5)
N1-C2	1.441(5)	C1-N1[1]	1.472(5)

[1]1/2-X,3/2-Y,+Z

Table S14. The bonds angles in **2**

Parameter	Bond angle (°)	Parameter	Bond length (Å)
C3-N3-C4	122.7(3)	O2A-N4-O1	111.7(8)
O4-N5-C5	118.4(3)	O2A-N4-C5	121.9(7)
O3-N5-O4	120.1(3)	N3-C3-C5	119.7(4)
O3-N5-C5	121.5 (3)	N2-C3-N3	117.4(3)
C2-N1-C1	111.8(2)	N2-C3-C5	122.9(3)
C4-N1-C1	114.6(3)	N5-C5-N4	116.5(3)
C4-N1-C2	108.7(3)	N5-C5-C3	123.2(3)
C3-N2-C2	122.5(3)	N4-C5-C3	120.1(3)
O1-N4-C5	120.4(4)	N1[1]-C1-N1	106.4(4)
O1-N4-O2	119.2(6)	N1-C2-N2	112.1(3)
O2-N4-C5	116.7(6)	N1-C4-N3	113.0(3)

Table S15. The torsion angles in **2**

Parameter	Torsion angle (°)	Parameter	Torsion angle (°)
C2-N1-C1-N1a	78.0(3)	O1-N4-C5-N5	-179.6(4)
C4-N1-C1-N1a	-157.8(3)	O1-N4-C5-C3	4.5(6)
C1-N1-C2-N2	75.4(4)	O2-N4-C5-N5	-21.3(8)
C4-N1-C2-N2	-52.1(4)	O2-N4-C5-C3	162.8(7)
C1-N1-C4-N3	-75.4(4)	O3-N5-C5-N4	7.0(5)
C2-N1-C4-N3	50.5(4)	O3-N5-C5-C3	-177.2(4)
C3-N2-C2-N1	32.2(5)	O4-N5-C5-N4	-171.4(3)
C2-N2-C3-N3	-7.4(6)	O4-N5-C5-C3	4.4(5)
C2-N2-C3-C5	175.6(3)	N2-C3-C5-N4	-1.3(6)
C4-N3-C3-N2	5.3(5)	N2-C3-C5-N5	-177.0(4)
C4-N3-C3-C5	-177.6(3)	N3-C3-C5-N4	-178.3(4)
C3-N3-C4-N1	-28.5(5)	N3-C3-C5-N5	6.1(6)

Table S16. The hydrogen bonds in **2**

D-H···A	D-H(Å)	H···A(Å)	D···A(Å)	D-H···A(o)
N2—H2···O1	0.8800	1.9100	2.567(4)	131.00
N2—H2···O3	0.8800	2.4900	3.263(5)	146.00
N3—H3···O4	0.8800	1.8900	2.556(4)	131.00
N3—H3···N5	0.8800	2.5300	2.882(5)	105.00
C2—H2A···N1	0.9900	2.6000	2.977(5)	102.00
C2—H2A···O2	0.9900	2.5400	3.309(12)	134.00
C4—H4A···O4	0.9900	2.3700	3.306(5)	158.00
C4—H4B···O2	0.9900	2.5500	3.226(10)	125.00

Table S17. The bonds length in **3**

Parameter	Bond length (Å)	Parameter	Bond length (Å)
O1-N2	1.232(4)	N3-C2	1.315(4)
O2-N2	1.237(4)	N3-C4	1.465(4)
O3-N1	1.234(4)	N4-C2	1.330(4)
O4-N1	1.225(4)	N4-C3	1.456(5)
O5-N7	1.204(5)	N5-C3	1.434(4)
O6-N7	1.189(5)	N5-C4	1.452(4)
O7-N6	1.202(5)	N5-C5	1.454(4)
O8-N6	1.215(5)	N6-C6	1.506(6)

O9-N8	1.193(6)	N7-C6	1.507(5)
O10-N8	1.211(5)	N8-C6	1.529(6)
N1-C1	1.397(5)	C1-C2	1.444(5)
N2-C1	1.403(4)	C5-C6	1.518(5)

Table S18. The bonds angles in **3**

Parameter	Bond angle (°)	Parameter	Bond length (Å)
O3-N1-C1	121.3(3)	O9-N8-C6	116.3(4)
O4-N1-O3	118.5(4)	O10-N8-C6	117.3(6)
O4-N1-C1	119.9(3)	N1-C1-N2	116.0(3)
O1-N2-O2	120.2(3)	N1-C1-C2	122.1(3)
O1-N2-C1	121.2(3)	N2-C1-C2	121.9(3)
O2-N2-C1	118.5(3)	N3-C2-N4	118.3(3)
C2-N3-C4	123.4(3)	N3-C2-C1	121.6(3)
C2-N4-C3	120.9(3)	N4-C2-C1	120.1(3)
C3-N5-C4	108.5(3)	N5-C3-N4	111.5(3)
C3-N5-C5	113.4(3)	N5-C4-N3	111.0(3)
C4-N5-C5	113.2(3)	N5-C5-C6	110.9(3)
O7-N6-O8	127.9(5)	N6-C6-N7	105.5(4)
O7-N6-C6	117.9(5)	N6-C6-N8	105.6(4)
O8-N6-C6	114.2(4)	N6-C6-C5	111.0(4)
O5-N7-C6	116.0(5)	N7-C6-N8	107.6(4)
O6-N7-O5	127.5(5)	N7-C6-C5	112.6(3)
O6-N7-C6	116.3(4)	C5-C6-N8	114.0(3)
O9-N8-O10	126.4(6)		

Table S19. The torsion angles in **3**

Parameter	Torsion angle (°)	Parameter	Torsion angle (°)
O1-N2-C1-N1	-22.9 (5)	O10-N8-C6-N6	-13.4(6)
O1-N2-C1-C2	155.3(3)	O10-N8-C6-N7	98.9(5)
O2-N2-C1-N1	159.7(4)	O10-N8-C6-C5	-135.5(5)
O2-N2-C1-C2	-22.0(5)	N1-C1-C2-N3	8.6(5)
O3-N1-C1-N2	-22.8(6)	N1-C1-C2-N4	-171.1(3)
O3-N1-C1-C2	158.9(4)	N2-C1-C2-N3	-169.5(3)
O4-N1-C1-N2	163.2(4)	N2-C1-C2-N4	10.7(5)
O4-N1-C1-C2	-15.0(6)	N5-C5-C6-N6	165.2(3)

O5-N7-C6-N6	109.2(6)	N5-C5-C6-N7	47.2(5)
O5-N7-C6-N8	-3.2(6)	N5-C5-C6-N8	-75.7(4)
O5-N7-C6-C5	-129.7(5)	C2-N3-C4-N5	23.2(5)
O6-N7-C6-N6	-75.1(5)	C2-N4-C3-N5	-33.9(4)
O6-N7-C6-N8	172.6(4)	C3-N4-C2-N3	3.4(5)
O6-N7-C6-C5	46.1(6)	C3-N4-C2-C1	-176.9(3)
O7-N6-C6-N7	-17.7(7)	C3-N5-C4-N3	-51.2(4)
O7-N6-C6-N8	96.1(6)	C3-N5-C5-C6	-115.5(3)
O7-N6-C6-C5	-139.9(6)	C4-N3-C2-N4	1.9(5)
O8-N6-C6-N7	163.7(5)	C4-N3-C2-C1	-177.9(3)
O8-N6-C6-N8	-82.5(6)	C4-N5-C3-N4	56.7(4)
O8-N6-C6-C5	41.6(6)	C4-N5-C5-C6	120.3(3)
O9-N8-C6-N6	167.5(5)	C5-N5-C3-N4	-70.0(4)
O9-N8-C6-N7	-80.1(6)	C5-N5-C4-N3	75.6(4)
O9-N8-C6-C5	45.4(6)		

Table S20. The hydrogen bonds in **3**

D-H···A	D-H(Å)	H···A(Å)	D···A(Å)	D-H···A(o)
N3—H3···O4	0.8800	1.9300	2.598(4)	131.00
N3—H3···N1	0.8800	2.5500	2.882(5)	103.00
N3—H3···O2	0.8800	2.4500	2.960(5)	118.00
N4—H4···O2	0.8800	1.9000	2.561(4)	131.00
N4—H4···N2	0.8800	2.5400	2.860(5)	103.00
N4—H4···O10	0.8800	2.4100	3.113(6)	138.00
C3—H3A···O7	0.9900	2.5400	3.307(6)	134.00
C3—H3B···O6	0.9900	2.3900	3.112(5)	129.00
C4—H4A···O9	0.9900	2.5800	3.140(6)	116.00
C4—H4B···O5	0.9900	2.3800	3.191(6)	139.00
C5—H5A···O4	0.9900	2.3400	3.312(5)	166.00
C5—H5B···O3	0.9900	2.3400	3.247(5)	152.00

II. Theoretical study

Theoretical calculations were performed by using the Gaussian 09 (Revision D.01) suite of programs.[1] Based on the method of isodesmic reactions (Scheme S1), gas-phase heats of formation of the neutral compounds were computed. The gas-phase enthalpies of the building-block molecules were obtained by using the atomization method with the G2 ab initio calculations. Then the remaining task is to determine the solid-state heats of formation for the synthesized compounds.

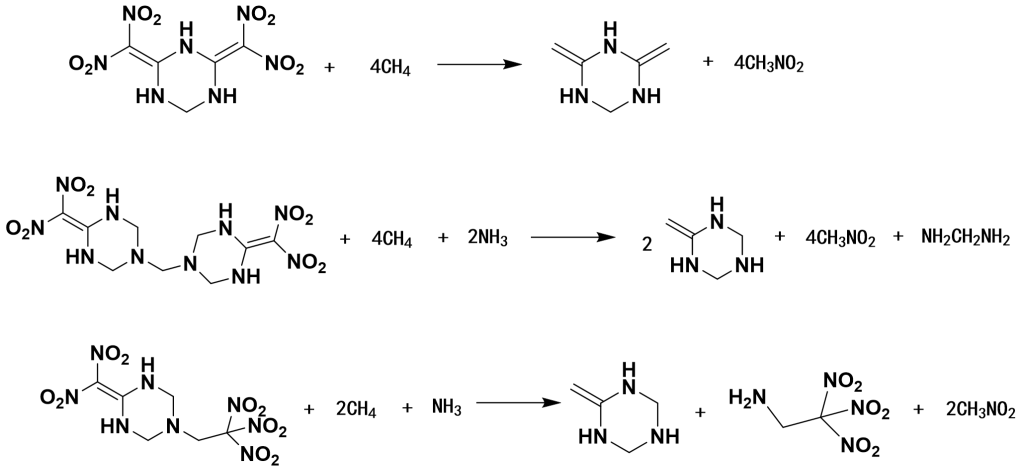
The solid-state enthalpy of formation for neutral compound can be estimated by subtracting the heat of sublimation from gas-phase heat of formation.

$$\Delta H_f = \Delta H_f(g) - \Delta H_{sub} \quad (1)$$

On the basis of the literature,[2] the heat of sublimation can be estimated with Trouton's rule according to eq 1, where T represents either the melting point or the decomposition temperature when no melting occurs prior to decomposition:

$$\Delta H_{sub} = 188/\text{J mol}^{-1}\text{K}^{-1} \times \text{T} \quad (2)$$

The detailed principle can be consulted from literatures[1-4].



Scheme S1. Isodesmic reactions

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