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Supporting Information

C-N Bonded Energetic Biheterocyclic Compounds with Good Detonation Performance and High Thermal Stability

Yongxing Tang,[a] Chunlin He,[a] Lauren A. Mitchell,[b] Damon A. Parrish[b] and Jean'ne M. Shreeve[a]

[a] Department of Chemistry, University of Idaho, Moscow, Idaho 83844-2343, United States
[b] Naval Research Laboratory, 4555 Overlook Avenue, Washington, D.C. 20375, United States

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Table S1 Crystal data and structure refinement for **4** and **7**

Identification code	**4**	**7**
CCDC No.	1434639	1434641
Empirical formula	$C_5H_4N_8O_7$	$C_6H_6N_{10}O_4$
Formula weight	288.16	282.21
Temperature/K	150(2)	150(2)
Wavelength/Å	0.71073	0.71073
Crystal system	Orthorhombic	Triclinic
Space group	$Pca2_1$	P-1
Unit cell dimensions	a = 16.562(9) Å□α = 90° b = 5.114(3) Å β = 90° c = 25.032(14) Å γ = 90°	a = 7.9947(7) Å□α = 79.297(2)° b = 9.0147(8) Å□β = 79.4120(10)° c = 16.5263(15) Å γ = 80.928(2)°
Volume/Å^3	2120(2)	1140.95(18)
Z	8	4
Density/Mg/m^3	1.805	1.643
Absorption coefficient/mm^{-1}	0.168	0.140
F(000)	1168	576
Crystal size/ mm^3	0.108 x 0.035 x 0.010	0.225 x 0.109 x 0.072
Theta range for data collection	2.591 to 28.967°	1.270 to 26.517°
Index ranges	-21<=h<=22, -6<=k<=6, -33<=l<=30	-10<=h<=10, -11<=k<=10, -20<=l<=20
Reflections collected	21718	10561
Data/restraints/parameters	5298/9/385	4682/1/375
Goodness-of-fit on F^2	0.894	1.073
Final R indices [I>2sigma(I)]	R_1 = 0.0447, wR_2 = 0.0770	R_1 = 0.0409, wR_2 = 0.1167
R indices (all data)	R_1 = 0.1055, wR_2 = 0.0984	R_1 = 0.0625, wR_2 = 0.1557
Largest diff. peak and hole/ e.Å^{-3}	0.312 and -0.281	0.533 and -0.399

Table S2 Crystal data and structure refinement for **9** and **11**

Identification code	**9**	**11**
CCDC No.	1434640	1434642
Empirical formula	$C_4H_5N_9O_4$	$C_5H_5N_9O_6$
Formula weight	243.17	287.18
Temperature/K	150	150(2)
Wavelength/Å	0.71073	0.71073
Crystal system	Orthorhombic	Monoclinic
Space group	$Pna2_1$	$P2_1/c$
Unit cell dimensions	a =13.9499(11) Å α = 90° b = 4.9380(4) Å β = 90° c = 13.2091(11) Å γ = 90°	a = 9.0972(8) Å□α = 90° b = 16.0829(14) Å β = 109.158(2)° c = 7.3453(7) Å γ = 90°
Volume/Å^3	909.90(13)	1015.17(16)
Z	4	4
Density/Mg/m^3	1.775	1.879
Absorption coefficient/mm^{-1}	0.156	0.170
F(000)	496.0	584
Crystal size/mm^3	0.3 × 0.15 × 0.15	0.119 x 0.061 x 0.060
Theta range for data collection	6.168 to 72.824°	3.198 to 26.459°

Index ranges	$-22 \le h \le 23$, $-8 \le k \le 8$, $-22 \le l \le 22$	-11<=h<=11, -20<=k<=20, -9<=l<=9
Reflections collected	51484	9247
Data/restraints/parameters	4428/1/174	2089/0/193
Goodness-of-fit on F^2	1.047	1.024
Final R indices [I>2sigma(I)]	$R_1 = 0.0418$, $wR_2 = 0.0825$	$R_1 = 0.0297$, $wR_2 = 0.0738$
R indices (all data)	$R_1 = 0.0593$, $wR_2 = 0.0886$	$R_1 = 0.0403$, $wR_2 = 0.0792$
Largest diff. peak and hole/ e.Å^{-3}	0.49/-0.24	0.322 and -0.214

Table S3 Bond lengths [Å] for **4**

O(1A)-N(3A)	1.227(6)	O(2A)-N(3A)	1.218(6)
N(3A)-C(5A)	1.460(6)	N(4A)-C(8A)	1.314(6)
N(4A)-C(5A)	1.346(6)	C(5A)-N(6A)	1.312(6)
C(5A)-C(8A)	2.026(7)	N(6A)-N(7A)	1.361(6)
N(7A)-C(8A)	1.332(6)	N(7A)-H(7A)	0.88(3)
C(8A)-N(9A)	1.394(6)	N(9A)-C(10A)	1.353(7)
N(9A)-N(13A)	1.359(5)	C(10A)-C(11A)	1.374(8)
C(10A)-H(10A)	0.95(6)	C(11A)-C(12A)	1.411(7)
C(11A)-N(14A)	1.444(7)	C(12A)-N(13A)	1.317(6)
C(12A)-N(17A)	1.455(6)	N(14A)-O(16A)	1.222(6)
N(14A)-O(15A)	1.226(6)	N(17A)-O(18A)	1.211(6)
N(17A)-O(19A)	1.222(6)	O(1SA)-H(1S)	0.79(3)
O(1SA)-H(2S)	0.81(3)	O(1B)-N(3B)	1.234(5)
O(2B)-N(3B)	1.215(6)	N(3B)-C(4B)	1.448(6)
C(4B)-N(6B)	1.320(6)	C(4B)-N(5B)	1.344(6)
C(4B)-C(8B)	2.028(7)	N(5B)-C(8B)	1.316(6)
N(6B)-N(7B)	1.357(6)	N(7B)-C(8B)	1.338(6)
N(7B)-H(7B)	0.89(3)	C(8B)-N(9B)	1.394(6)
N(9B)-C(10B)	1.354(7)	N(9B)-N(13B)	1.359(6)
C(10B)-C(11B)	1.360(8)	C(10B)-H(10B)	0.93(6)
C(11B)-C(12B)	1.404(7)	C(11B)-N(14B)	1.449(7)
C(12B)-N(13B)	1.317(7)	C(12B)-N(17B)	1.453(7)
N(14B)-O(16B)	1.213(6)	N(14B)-O(15B)	1.229(5)
N(17B)-O(19B)	1.225(6)	N(17B)-O(18B)	1.230(6)
O(1SB)-H(3S)	0.80(3)	O(1SB)-H(4S)	0.82(3)

Table S4 Bond angles [°] for **4**

O(2A)-N(3A)-O(1A)	125.4(4)	O(2A)-N(3A)-C(5A)	117.1(4)
O(1A)-N(3A)-C(5A)	117.5(4)	C(8A)-N(4A)-C(5A)	99.2(4)
N(6A)-C(5A)-N(4A)	118.2(4)	N(6A)-C(5A)-N(3A)	119.1(4)
N(4A)-C(5A)-N(3A)	122.7(4)	N(6A)-C(5A)-C(8A)	78.4(3)
N(4A)-C(5A)-C(8A)	39.8(3)	N(3A)-C(5A)-C(8A)	162.4(4)
C(5A)-N(6A)-N(7A)	101.0(4)	C(8A)-N(7A)-N(6A)	108.1(4)
C(8A)-N(7A)-H(7A)	134(4)	N(6A)-N(7A)-H(7A)	118(4)
N(4A)-C(8A)-N(7A)	113.5(4)	N(4A)-C(8A)-N(9A)	125.3(5)
N(7A)-C(8A)-N(9A)	121.2(4)	N(4A)-C(8A)-C(5A)	41.0(3)
N(7A)-C(8A)-C(5A)	72.5(3)	N(9A)-C(8A)-C(5A)	166.2(4)
C(10A)-N(9A)-N(13A)	114.1(4)	C(10A)-N(9A)-C(8A)	127.4(4)
N(13A)-N(9A)-C(8A)	118.4(4)	N(9A)-C(10A)-C(11A)	105.1(5)

N(9A)-C(10A)-H(10A)	127(3)	C(11A)-C(10A)-H(10A)	128(3)
C(10A)-C(11A)-C(12A)	105.1(5)	C(10A)-C(11A)-N(14A)	122.8(5)
C(12A)-C(11A)-N(14A)	132.0(5)	N(13A)-C(12A)-C(11A)	112.6(4)
N(13A)-C(12A)-N(17A)	116.7(5)	C(11A)-C(12A)-N(17A)	130.5(5)
C(12A)-N(13A)-N(9A)	103.1(4)	O(16A)-N(14A)-O(15A)	125.2(5)
O(16A)-N(14A)-C(11A)	118.3(5)	O(15A)-N(14A)-C(11A)	116.5(4)
O(18A)-N(17A)-O(19A)	125.4(5)	O(18A)-N(17A)-C(12A)	117.2(5)
O(19A)-N(17A)-C(12A)	117.4(4)	H(1S)-O(1SA)-H(2S)	97(4)
O(2B)-N(3B)-O(1B)	124.8(4)	O(2B)-N(3B)-C(4B)	118.1(4)
O(1B)-N(3B)-C(4B)	117.1(4)	N(6B)-C(4B)-N(5B)	118.1(5)
N(6B)-C(4B)-N(3B)	119.4(4)	N(5B)-C(4B)-N(3B)	122.5(4)
N(6B)-C(4B)-C(8B)	78.3(3)	N(5B)-C(4B)-C(8B)	39.8(3)
N(3B)-C(4B)-C(8B)	162.2(4)	C(8B)-N(5B)-C(4B)	99.3(4)
C(4B)-N(6B)-N(7B)	101.1(4)	C(8B)-N(7B)-N(6B)	108.2(4)
C(8B)-N(7B)-H(7B)	135(4)	N(6B)-N(7B)-H(7B)	116(4)
N(5B)-C(8B)-N(7B)	113.4(4)	N(5B)-C(8B)-N(9B)	124.8(5)
N(7B)-C(8B)-N(9B)	121.8(4)	N(5B)-C(8B)-C(4B)	40.8(3)
N(7B)-C(8B)-C(4B)	72.5(3)	N(9B)-C(8B)-C(4B)	165.7(4)
C(10B)-N(9B)-N(13B)	113.9(4)	C(10B)-N(9B)-C(8B)	128.0(4)
N(13B)-N(9B)-C(8B)	118.1(4)	N(9B)-C(10B)-C(11B)	105.0(5)
N(9B)-C(10B)-H(10B)	121(4)	C(11B)-C(10B)-H(10B)	134(4)
C(10B)-C(11B)-C(12B)	105.9(5)	C(10B)-C(11B)-N(14B)	125.0(5)
C(12B)-C(11B)-N(14B)	128.9(5)	N(13B)-C(12B)-C(11B)	112.1(4)
N(13B)-C(12B)-N(17B)	118.5(5)	C(11B)-C(12B)-N(17B)	129.2(5)
C(12B)-N(13B)-N(9B)	103.1(4)	O(16B)-N(14B)-O(15B)	124.5(5)
O(16B)-N(14B)-C(11B)	118.8(5)	O(15B)-N(14B)-C(11B)	116.7(5)
O(19B)-N(17B)-O(18B)	125.8(5)	O(19B)-N(17B)-C(12B)	117.9(5)
O(18B)-N(17B)-C(12B)	116.3(5)	H(3S)-O(1SB)-H(4S)	92(3)

Table S5 Hydrogen bonds for **4** [Å and °]

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1SA)-H(1S)...O(2A)#1	0.79(3)	2.22(3)	2.989(5)	166(6)
O(1SA)-H(2S)...N(6B)#2	0.81(3)	2.11(3)	2.904(6)	166(6)
O(1SB)-H(3S)...O(1B)#3	0.80(3)	2.22(3)	3.015(5)	173(6)
O(1SB)-H(4S)...O(2A)#4	0.82(3)	2.58(5)	3.150(5)	128(5)
O(1SB)-H(4S)...N(6A)#4	0.82(3)	2.14(3)	2.923(6)	159(5)
N(7A)-H(7A)...O(1SA)	0.88(3)	1.79(3)	2.667(6)	174(7)
N(7B)-H(7B)...O(1SB)	0.89(3)	1.78(3)	2.664(6)	178(6)
C(10A)-H(10A)...O(15B)#5	0.95(6)	2.41(6)	3.208(7)	142(5)
C(10B)-H(10B)...O(16A)	0.93(6)	2.34(6)	3.210(7)	156(5)

Symmetry transformations used to generate equivalent atoms:
#1 x-1/2,-y+1,z #2 -x+1,-y,z+1/2 #3 x-1/2,-y,z
#4 -x+1,-y,z-1/2 #5 x+1/2,-y+2,z

Table S6 Bond lengths [Å] for **7**

N(1)-C(5)	1.354(3)	N(1)-N(2)	1.365(2)

N(1)-C(6)	1.406(3)	N(2)-C(3)	1.312(3)
C(3)-N(4)	1.348(3)	C(3)-N(11)	1.456(3)
N(4)-C(5)	1.315(3)	C(5)-H(5)	0.9500
C(6)-N(10)	1.321(3)	C(6)-N(7)	1.344(3)
N(7)-N(8)	1.353(2)	N(7)-N(14)	1.391(3)
N(8)-C(9)	1.319(3)	C(9)-N(10)	1.346(3)
C(9)-N(15)	1.452(3)	N(11)-O(12)	1.221(3)
N(11)-O(13)	1.222(3)	N(14)-H(14B)	0.91(3)
N(14)-H(14A)	0.83(3)	N(15)-O(17)	1.222(2)
N(15)-O(16)	1.226(2)	N(18)-N(19)	1.361(2)
N(18)-C(22)	1.366(3)	N(18)-C(23)	1.399(3)
N(19)-C(20)	1.307(3)	C(20)-N(21)	1.348(3)
C(20)-N(28)	1.453(3)	N(21)-C(22)	1.312(3)
C(22)-H(22)	0.9500	C(23)-N(27)	1.318(3)
C(23)-N(24)	1.345(3)	N(24)-N(25)	1.365(2)
N(24)-N(31)	1.395(2)	N(25)-C(26)	1.316(3)
C(26)-N(27)	1.344(3)	C(26)-N(32)	1.455(3)
N(28)-O(29)	1.223(2)	N(28)-O(30)	1.229(2)
N(31)-H(31A)	0.93(3)	N(31)-H(31B)	0.920(18)
N(32)-O(33)	1.221(2)	N(32)-O(34)	1.229(2)
N(1S)-C(2S)	1.138(4)	N(4S)-C(5S)	1.142(3)
C(5S)-C(6S)	1.453(3)	C(6S)-H(6S)	0.9800
C(6S)-H(4S)	0.9800	C(6S)-H(5S)	0.9800
C(2S)-C(3S)	1.445(4)	C(3S)-H(1S)	0.9800
C(3S)-H(3S)	0.9800	C(3S)-H(2S)	0.9800

Table S7 Bond angles [°] for **7**

C(5)-N(1)-N(2)	110.16(17)	C(5)-N(1)-C(6)	128.88(18)
N(2)-N(1)-C(6)	120.96(17)	C(3)-N(2)-N(1)	100.15(17)
N(2)-C(3)-N(4)	117.94(19)	N(2)-C(3)-N(11)	119.7(2)
N(4)-C(3)-N(11)	122.32(19)	C(5)-N(4)-C(3)	101.54(18)
N(4)-C(5)-N(1)	110.21(19)	N(4)-C(5)-H(5)	124.9
N(1)-C(5)-H(5)	124.9	N(10)-C(6)-N(7)	111.91(18)
N(10)-C(6)-N(1)	124.79(18)	N(7)-C(6)-N(1)	123.27(19)
C(6)-N(7)-N(8)	109.26(17)	C(6)-N(7)-N(14)	130.53(17)
N(8)-N(7)-N(14)	119.98(16)	C(9)-N(8)-N(7)	100.77(16)
N(8)-C(9)-N(10)	118.03(18)	N(8)-C(9)-N(15)	121.19(18)
N(10)-C(9)-N(15)	120.77(19)	C(6)-N(10)-C(9)	100.01(17)
O(12)-N(11)-O(13)	125.4(2)	O(12)-N(11)-C(3)	117.48(19)
O(13)-N(11)-C(3)	117.1(2)	N(7)-N(14)-H(14B)	104(2)
N(7)-N(14)-H(14A)	110(2)	H(14B)-N(14)-H(14A)	107(3)
O(17)-N(15)-O(16)	124.93(19)	O(17)-N(15)-C(9)	117.12(18)
O(16)-N(15)-C(9)	117.95(18)	N(19)-N(18)-C(22)	110.17(16)
N(19)-N(18)-C(23)	117.97(16)	C(22)-N(18)-C(23)	131.72(18)
C(20)-N(19)-N(18)	100.26(16)	N(19)-C(20)-N(21)	118.09(18)
N(19)-C(20)-N(28)	120.26(18)	N(21)-C(20)-N(28)	121.64(17)
C(22)-N(21)-C(20)	101.83(16)	N(21)-C(22)-N(18)	109.64(18)
N(21)-C(22)-H(22)	125.2	N(18)-C(22)-H(22)	125.2
N(27)-C(23)-N(24)	111.68(18)	N(27)-C(23)-N(18)	123.15(18)
N(24)-C(23)-N(18)	125.17(18)	C(23)-N(24)-N(25)	109.36(17)

C(23)-N(24)-N(31)	127.13(18)	N(25)-N(24)-N(31)	123.39(17)
C(26)-N(25)-N(24)	100.21(16)	N(25)-C(26)-N(27)	118.39(18)
N(25)-C(26)-N(32)	120.65(18)	N(27)-C(26)-N(32)	120.96(18)
C(23)-N(27)-C(26)	100.35(17)	O(29)-N(28)-O(30)	125.50(18)
O(29)-N(28)-C(20)	118.19(16)	O(30)-N(28)-C(20)	116.31(17)
N(24)-N(31)-H(31A)	105.1(19)	N(24)-N(31)-H(31B)	107(2)
H(31A)-N(31)-H(31B)	108(3)	O(33)-N(32)-O(34)	125.54(18)
O(33)-N(32)-C(26)	116.81(17)	O(34)-N(32)-C(26)	117.64(17)
N(4S)-C(5S)-C(6S)	178.4(3)	C(5S)-C(6S)-H(6S)	109.5
C(5S)-C(6S)-H(4S)	109.5	H(6S)-C(6S)-H(4S)	109.5
C(5S)-C(6S)-H(5S)	109.5	H(6S)-C(6S)-H(5S)	109.5
H(4S)-C(6S)-H(5S)	109.5	N(1S)-C(2S)-C(3S)	179.6(3)
C(2S)-C(3S)-H(1S)	109.5	C(2S)-C(3S)-H(3S)	109.5
H(1S)-C(3S)-H(3S)	109.5	C(2S)-C(3S)-H(2S)	109.5
H(1S)-C(3S)-H(2S)	109.5	H(3S)-C(3S)-H(2S)	109.5

Table S8 Torsion angles [°] for **7**

C(5)-N(1)-N(2)-C(3)	0.7(2)	C(23)-N(18)-N(19)-C(20)	-176.81(17)
C(6)-N(1)-N(2)-C(3)	-179.00(18)	N(18)-N(19)-C(20)-N(21)	0.5(2)
N(1)-N(2)-C(3)-N(4)	-0.2(2)	N(18)-N(19)-C(20)-N(28)	-178.83(18)
N(1)-N(2)-C(3)-N(11)	179.52(18)	N(19)-C(20)-N(21)-C(22)	-0.2(3)
N(2)-C(3)-N(4)-C(5)	-0.3(3)	N(28)-C(20)-N(21)-C(22)	179.17(19)
N(11)-C(3)-N(4)-C(5)	179.9(2)	C(20)-N(21)-C(22)-N(18)	-0.3(2)
C(3)-N(4)-C(5)-N(1)	0.7(2)	N(19)-N(18)-C(22)-N(21)	0.6(2)
N(2)-N(1)-C(5)-N(4)	-1.0(3)	C(23)-N(18)-C(22)-N(21)	176.1(2)
C(6)-N(1)-C(5)-N(4)	178.7(2)	N(19)-N(18)-C(23)-N(27)	1.7(3)
C(5)-N(1)-C(6)-N(10)	-50.2(3)	C(22)-N(18)-C(23)-N(27)	-173.5(2)
N(2)-N(1)-C(6)-N(10)	129.5(2)	N(19)-N(18)-C(23)-N(24)	-178.08(19)
C(5)-N(1)-C(6)-N(7)	127.8(2)	C(22)-N(18)-C(23)-N(24)	6.7(4)
N(2)-N(1)-C(6)-N(7)	-52.6(3)	N(27)-C(23)-N(24)-N(25)	0.6(2)
N(10)-C(6)-N(7)-N(8)	-1.3(2)	N(18)-C(23)-N(24)-N(25)	-179.62(19)
N(1)-C(6)-N(7)-N(8)	-179.49(17)	N(27)-C(23)-N(24)-N(31)	176.7(2)
N(10)-C(6)-N(7)-N(14)	173.02(19)	N(18)-C(23)-N(24)-N(31)	-3.5(3)
N(1)-C(6)-N(7)-N(14)	-5.2(3)	C(23)-N(24)-N(25)-C(26)	-0.6(2)
C(6)-N(7)-N(8)-C(9)	1.2(2)	N(31)-N(24)-N(25)-C(26)	-176.8(2)
N(14)-N(7)-N(8)-C(9)	-173.83(18)	N(24)-N(25)-C(26)-N(27)	0.5(2)
N(7)-N(8)-C(9)-N(10)	-0.8(2)	N(24)-N(25)-C(26)-N(32)	-179.41(18)
N(7)-N(8)-C(9)-N(15)	178.90(17)	N(24)-C(23)-N(27)-C(26)	-0.3(2)
N(7)-C(6)-N(10)-C(9)	0.7(2)	N(18)-C(23)-N(27)-C(26)	179.92(19)
N(1)-C(6)-N(10)-C(9)	178.90(19)	N(25)-C(26)-N(27)-C(23)	-0.1(2)
N(8)-C(9)-N(10)-C(6)	0.1(2)	N(32)-C(26)-N(27)-C(23)	179.73(18)
N(15)-C(9)-N(10)-C(6)	-179.63(17)	N(19)-C(20)-N(28)-O(29)	0.1(3)
N(2)-C(3)-N(11)-O(12)	2.7(3)	N(21)-C(20)-N(28)-O(29)	-179.16(18)
N(4)-C(3)-N(11)-O(12)	-177.5(2)	N(19)-C(20)-N(28)-O(30)	179.85(18)
N(2)-C(3)-N(11)-O(13)	-177.4(2)	N(21)-C(20)-N(28)-O(30)	0.5(3)
N(4)-C(3)-N(11)-O(13)	2.4(3)	N(25)-C(26)-N(32)-O(33)	-171.6(2)
N(8)-C(9)-N(15)-O(17)	-148.9(2)	N(27)-C(26)-N(32)-O(33)	8.5(3)
N(10)-C(9)-N(15)-O(17)	30.8(3)	N(25)-C(26)-N(32)-O(34)	9.3(3)
N(8)-C(9)-N(15)-O(16)	31.3(3)	N(27)-C(26)-N(32)-O(34)	-170.61(19)
N(10)-C(9)-N(15)-O(16)	-149.0(2)		
C(22)-N(18)-N(19)-C(20)	-0.6(2)		

Table S9 Hydrogen bonds for **7** [Å and °]

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(5)-H(5)...O(30)	0.95	2.40	3.169(3)	138.2
C(22)-H(22)...N(31)	0.95	2.50	3.014(3)	114.1
C(22)-H(22)...N(4S)#1	0.95	2.43	3.282(3)	148.5
C(6S)-H(5S)...O(13)#2	0.98	2.54	3.202(3)	124.5
C(3S)-H(2S)...O(12)#3	0.98	2.51	3.402(3)	151.4
N(14)-H(14B)...N(21)#4	0.91(3)	2.34(4)	3.222(3)	164(3)
N(14)-H(14A)...N(19)#5	0.83(3)	2.49(3)	3.208(3)	146(3)
N(14)-H(14A)...N(27)#5	0.83(3)	2.32(3)	3.032(3)	144(3)
N(31)-H(31A)...N(1S)	0.93(3)	2.16(3)	3.091(3)	173(3)
N(31)-H(31B)...O(16)#6	0.920(18)	2.60(3)	3.074(3)	113(2)

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,-y,-z #2 -x+2,-y,-z+1 #3 x,y,z-1
#4 -x+1,-y+1,-z+1 #5 -x+2,-y+1,-z+1 #6 x,y-1,z

Table S10 Bond Lengths for **9**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	N1	1.2240(18)	N4	C2	1.3541(19)
O2	N1	1.2166(18)	N4	C3	1.4083(18)
O3	N8	1.2275(18)	N5	C3	1.3326(19)
O4	N8	1.2248(18)	N5	C4	1.3410(19)
N1	C1	1.4534(19)	N6	N7	1.3687(18)
N2	C1	1.3454(19)	N6	C3	1.3305(18)
N2	C2	1.325(2)	N7	C4	1.3225(19)
N3	N4	1.3599(16)	N8	C4	1.4449(19)
N3	C1	1.3106(19)			

Table S11 Bond Angles for **9**

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	N1	C1	116.77(13)	O4	N8	O3	124.78(14)
O2	N1	O1	125.48(13)	O4	N8	C4	117.46(13)
O2	N1	C1	117.72(13)	N2	C1	N1	121.22(12)
C2	N2	C1	101.39(12)	N3	C1	N1	120.34(12)
C1	N3	N4	100.04(12)	N3	C1	N2	118.25(13)
N3	N4	C3	120.11(11)	N2	C2	N4	109.65(13)
C2	N4	N3	110.67(12)	N5	C3	N4	121.94(13)
C2	N4	C3	129.03(12)	N6	C3	N4	121.68(12)
C3	N5	C4	98.26(12)	N6	C3	N5	116.37(13)
C3	N6	N7	104.53(12)	N5	C4	N8	121.44(13)
C4	N7	N6	103.96(12)	N7	C4	N5	116.88(13)
O3	N8	C4	117.77(13)	N7	C4	N8	121.68(12)

Table S12 Hydrogen Bonds for **9**

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N9	H9A	N5	0.87(3)	2.09(3)	2.9566(19)	179(2)
N9	H9B	N6[1]	0.86(2)	2.14(2)	2.927(2)	152(2)
N9	H9C	N7[2]	0.85(2)	2.22(2)	3.0073(19)	155(2)
N9	H9D	N2[3]	0.82(3)	2.25(3)	3.0751(19)	175(3)

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

Table S13 Torsion Angles for **9**

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O1	N1	C1	N2	-4.6(2)	N7	N6	C3	N4	-179.16(13)
O1	N1	C1	N3	-179.49(14)	N7	N6	C3	N5	-0.52(18)
O2	N1	C1	N2	173.61(14)	C1	N2	C2	N4	-0.02(18)
O2	N1	C1	N3	-1.3(2)	C1	N3	N4	C2	0.22(16)
O3	N8	C4	N5	176.63(14)	C1	N3	N4	C3	-175.08(12)
O3	N8	C4	N7	-3.5(2)	C2	N2	C1	N1	-174.82(14)
O4	N8	C4	N5	-3.4(2)	C2	N2	C1	N3	0.19(19)
O4	N8	C4	N7	176.43(14)	C2	N4	C3	N5	160.54(15)
N3	N4	C2	N2	-0.13(19)	C2	N4	C3	N6	-20.9(2)
N3	N4	C3	N5	-25.1(2)	C3	N4	C2	N2	174.63(14)
N3	N4	C3	N6	153.44(14)	C3	N5	C4	N7	0.27(18)
N4	N3	C1	N1	174.80(13)	C3	N5	C4	N8	-179.86(12)
N4	N3	C1	N2	-0.26(17)	C3	N6	N7	C4	0.60(15)
N6	N7	C4	N5	-0.58(18)	C4	N5	C3	N4	178.81(12)
N6	N7	C4	N8	179.55(13)	C4	N5	C3	N6	0.18(17)

Table S14 Bond lengths [Å] and angles [°] for **11**

N(1)-C(5)	1.3202(18)	C(9)-N(14)	1.4533(18)
N(1)-C(2)	1.3515(18)	C(10)-N(17)	1.4273(18)
C(2)-N(3)	1.3044(19)	N(11)-O(13)	1.2201(17)
C(2)-N(11)	1.4572(18)	N(11)-O(12)	1.2273(16)
N(3)-N(4)	1.3667(16)	N(14)-O(15)	1.2235(16)
N(4)-C(5)	1.3569(18)	N(14)-O(16)	1.2333(16)
N(4)-C(6)	1.4180(18)	N(17)-O(19)	1.2264(16)
C(5)-H(5)	0.9500	N(17)-O(18)	1.2356(17)
C(6)-N(7)	1.3385(19)	N(1S)-H(2S)	0.89(2)
C(6)-C(10)	1.388(2)	N(1S)-H(1S)	0.88(2)
N(7)-N(8)	1.3706(16)	N(1S)-H(4S)	0.87(2)
N(8)-C(9)	1.3269(19)	N(1S)-H(3S)	0.90(2)
C(9)-C(10)	1.3980(19)		

C(5)-N(1)-C(2)	101.62(12)
N(3)-C(2)-N(1)	117.81(13)
N(3)-C(2)-N(11)	120.37(12)
N(1)-C(2)-N(11)	121.81(12)
C(2)-N(3)-N(4)	100.64(11)
C(5)-N(4)-N(3)	109.96(11)
C(5)-N(4)-C(6)	130.18(12)
N(3)-N(4)-C(6)	119.24(11)
N(1)-C(5)-N(4)	109.95(12)
N(1)-C(5)-H(5)	125.0
N(4)-C(5)-H(5)	125.0
N(7)-C(6)-C(10)	110.90(12)
N(7)-C(6)-N(4)	119.03(13)
C(10)-C(6)-N(4)	130.04(13)
C(6)-N(7)-N(8)	107.93(12)
C(9)-N(8)-N(7)	107.02(11)
N(8)-C(9)-C(10)	111.74(12)
N(8)-C(9)-N(14)	120.03(12)
C(10)-C(9)-N(14)	127.60(13)
C(6)-C(10)-C(9)	102.39(12)
C(6)-C(10)-N(17)	127.96(13)
C(9)-C(10)-N(17)	128.70(13)
O(13)-N(11)-O(12)	125.59(13)
O(13)-N(11)-C(2)	117.59(12)
O(12)-N(11)-C(2)	116.81(12)
O(15)-N(14)-O(16)	124.73(12)
O(15)-N(14)-C(9)	118.40(12)
O(16)-N(14)-C(9)	116.83(11)
O(19)-N(17)-O(18)	124.15(13)
O(19)-N(17)-C(10)	118.19(12)
O(18)-N(17)-C(10)	117.65(12)
H(2S)-N(1S)-H(1S)	110.6(17)
H(2S)-N(1S)-H(4S)	107.3(17)
H(1S)-N(1S)-H(4S)	111.1(17)
H(2S)-N(1S)-H(3S)	109.7(16)
H(1S)-N(1S)-H(3S)	110.0(16)
H(4S)-N(1S)-H(3S)	108.0(18)

Table S15 Torsion angles [°] for **11**

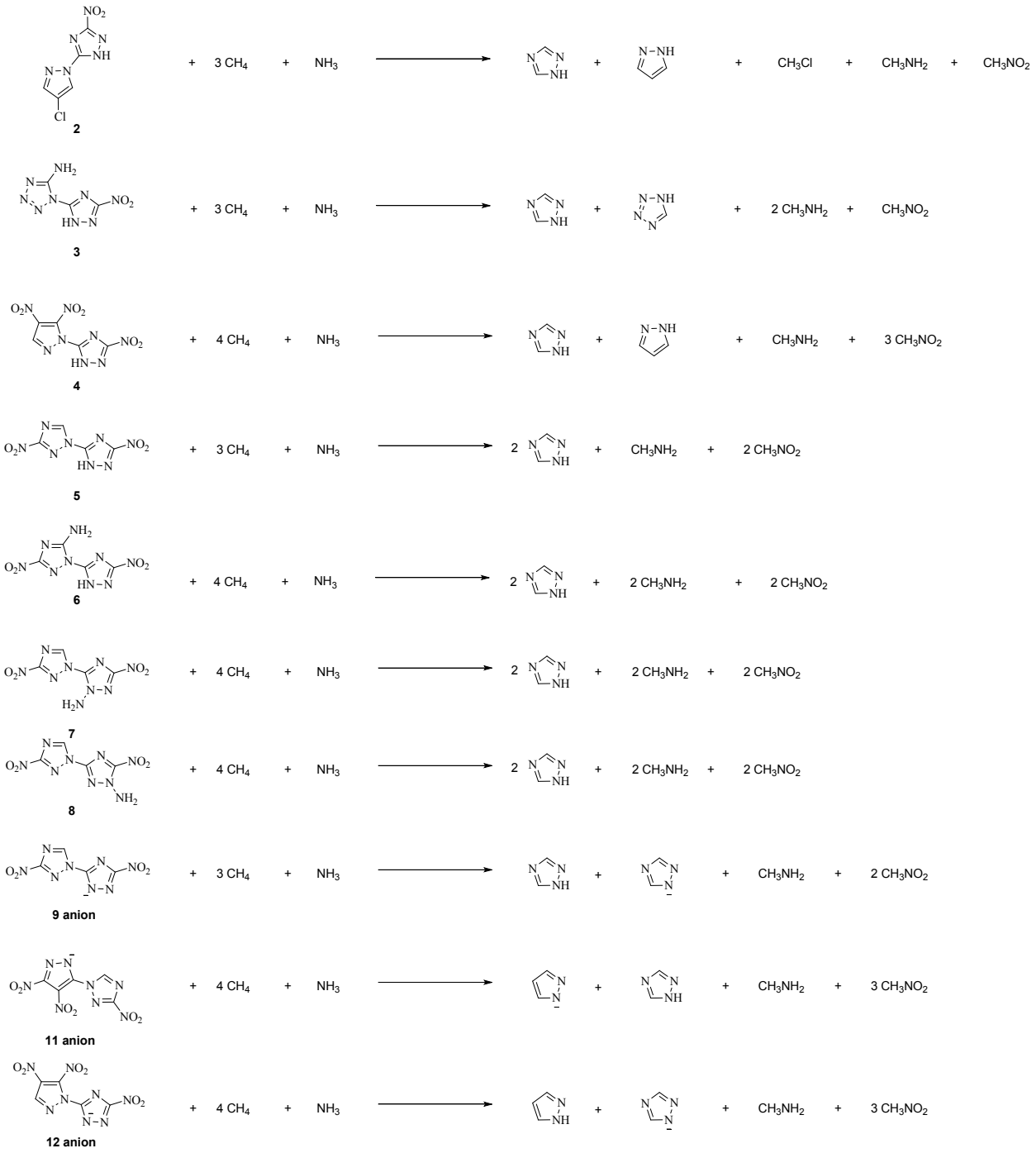
C(5)-N(1)-C(2)-N(3)	-1.21(17)
C(5)-N(1)-C(2)-N(11)	179.57(13)
N(1)-C(2)-N(3)-N(4)	1.18(16)
N(11)-C(2)-N(3)-N(4)	-179.59(12)
C(2)-N(3)-N(4)-C(5)	-0.65(15)
C(2)-N(3)-N(4)-C(6)	-172.52(12)
C(2)-N(1)-C(5)-N(4)	0.66(15)
N(3)-N(4)-C(5)-N(1)	-0.02(16)
C(6)-N(4)-C(5)-N(1)	170.68(13)
C(5)-N(4)-C(6)-N(7)	-119.39(16)
N(3)-N(4)-C(6)-N(7)	50.59(18)
C(5)-N(4)-C(6)-C(10)	62.5(2)

N(3)-N(4)-C(6)-C(10)	-127.57(16)
C(10)-C(6)-N(7)-N(8)	-1.50(16)
N(4)-C(6)-N(7)-N(8)	-179.99(11)
C(6)-N(7)-N(8)-C(9)	1.34(15)
N(7)-N(8)-C(9)-C(10)	-0.72(16)
N(7)-N(8)-C(9)-N(14)	-172.24(11)
N(7)-C(6)-C(10)-C(9)	1.02(15)
N(4)-C(6)-C(10)-C(9)	179.29(14)
N(7)-C(6)-C(10)-N(17)	-168.52(13)
N(4)-C(6)-C(10)-N(17)	9.7(2)
N(8)-C(9)-C(10)-C(6)	-0.16(16)
N(14)-C(9)-C(10)-C(6)	170.57(13)
N(8)-C(9)-C(10)-N(17)	169.28(13)
N(14)-C(9)-C(10)-N(17)	-20.0(2)
N(3)-C(2)-N(11)-O(13)	4.7(2)
N(1)-C(2)-N(11)-O(13)	-176.14(14)
N(3)-C(2)-N(11)-O(12)	-174.26(13)
N(1)-C(2)-N(11)-O(12)	4.9(2)
N(8)-C(9)-N(14)-O(15)	-31.01(19)
C(10)-C(9)-N(14)-O(15)	158.94(14)
N(8)-C(9)-N(14)-O(16)	146.77(13)
C(10)-C(9)-N(14)-O(16)	-23.3(2)
C(6)-C(10)-N(17)-O(19)	-37.1(2)
C(9)-C(10)-N(17)-O(19)	156.02(14)
C(6)-C(10)-N(17)-O(18)	141.87(15)
C(9)-C(10)-N(17)-O(18)	-25.0(2)

Table S16 Hydrogen bonds for **11** [Å and °]

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(5)-H(5)...N(8)#1	0.95	2.59	3.2870(19)	130.8
C(5)-H(5)...O(15)#1	0.95	2.29	3.1880(18)	157.4
N(1S)-H(2S)...O(12)#2	0.89(2)	2.566(18)	3.1149(18)	120.8(14)
N(1S)-H(2S)...O(18)#3	0.89(2)	2.13(2)	2.9663(18)	157.1(16)
N(1S)-H(1S)...N(1)	0.88(2)	2.10(2)	2.9760(18)	171.7(17)
N(1S)-H(4S)...N(7)#4	0.87(2)	2.14(2)	2.9796(19)	161.5(17)
N(1S)-H(3S)...N(8)#5	0.90(2)	2.35(2)	3.0801(19)	137.9(15)
N(1S)-H(3S)...O(13)#6	0.90(2)	2.585(18)	3.1172(18)	118.6(15)

Symmetry transformations used to generate equivalent atoms:
#1 x,-y+3/2,z+1/2 #2 x,-y+1/2,z+1/2 #3 -x+2,-y+1,-z+2
#4 -x+1,-y+1,-z+1 #5 -x+1,y-1/2,-z+3/2 #6 x,y,z+1



Scheme S1 Isodesmic reactions for the synthesized compounds