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Electronic Supplementary Information

Aminoacetonitrile as Precursor for Nitrogen Rich Stable and Insensitive Asymmetric N-Methylene-C Linked Tetrazole-Based Energetic Compounds

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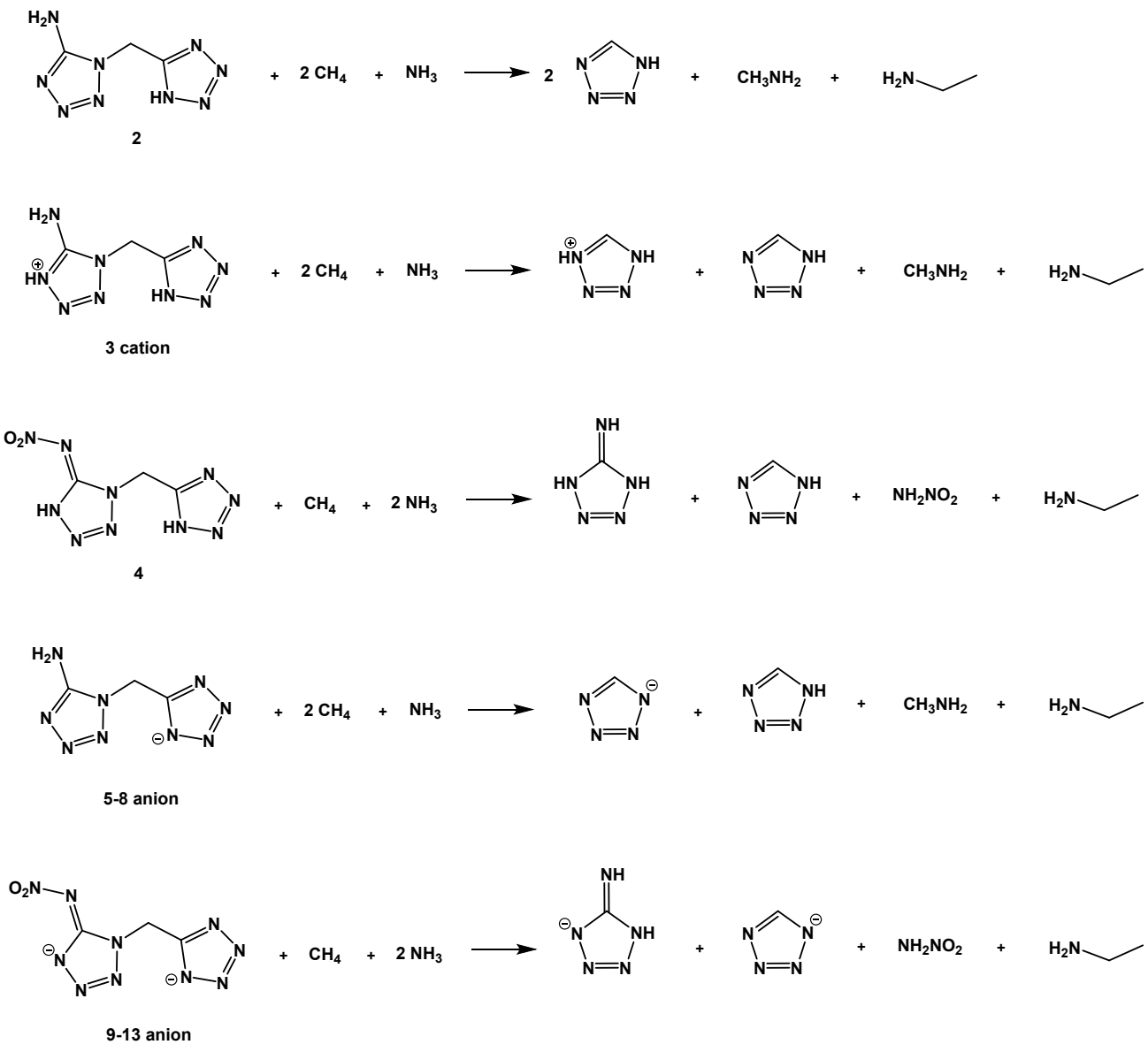
1. Isodesmic Reactions



Scheme S1: Isodesmic reactions for the compounds **2 - 13**

3. Crystal Structure Data

Table S1. Crystal data and structure refinement for Compound **2**.

Identification code	shrv413	
Empirical formula	$C_3H_5N_9$	
Formula weight	167.16	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 4.940(3) Å	α= 97.538(9)°.
	b = 5.906(4) Å	β= 90.277(8)°.
	c = 12.109(7) Å	γ = 105.359(9)°.
Volume	337.5(3) $Å^3$	
Z	2	
Density (-123°C)	1.645 Mg/m^3	
Density (20°C)	1.616 Mg/m^3	
Absorption coefficient	0.127 mm^{-1}	
F(000)	172	
Crystal size	0.200 x 0.150 x 0.030 mm^3	
Theta range for data collection	1.698 to 26.066°.	
Index ranges	-6<=h<=6, -7<=k<=7, 0<=l<=14	
Reflections collected	1164	
Independent reflections	1164 [R_{int} = 0.0218]	
Completeness to theta = 25.242°	91.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.745370 and 0.641986	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1164 / 2 / 116	
Goodness-of-fit on F^2	1.106	
Final R indices [I>2sigma(I)]	R_1 = 0.0293, wR_2 = 0.0676	
R indices (all data)	R_1 = 0.0332, wR_2 = 0.0725	
Largest diff. peak and hole	0.187 and -0.198 $e.Å^{-3}$	
CCDC No	1554453	

Table S2. Bond lengths [Å] and angles [°] for Compound **2**.

N(1)-C(2)	1.326(3)
C(2)-N(3)	1.336(2)
C(2)-N(6)	1.351(2)
N(4)-N(5)	1.288(2)
N(4)-N(3)	1.361(3)
N(6)-N(5)	1.364(2)

N(6)-C(7)	1.458(2)
C(7)-C(8)	1.498(3)
C(8)-N(12)	1.317(2)
C(8)-N(9)	1.336(2)
N(9)-N(10)	1.344(2)
N(11)-N(10)	1.296(2)
N(11)-N(12)	1.367(2)

N(1)-C(2)-N(3)	126.09(18)
N(1)-C(2)-N(6)	126.09(17)
N(3)-C(2)-N(6)	107.82(18)
N(5)-N(4)-N(3)	112.51(16)
C(2)-N(3)-N(4)	105.36(16)
C(2)-N(6)-N(5)	108.91(15)
C(2)-N(6)-C(7)	129.91(17)
N(5)-N(6)-C(7)	120.78(15)
N(4)-N(5)-N(6)	105.39(16)
N(6)-C(7)-C(8)	110.07(15)
N(12)-C(8)-N(9)	108.75(16)
N(12)-C(8)-C(7)	124.85(15)
N(9)-C(8)-C(7)	126.36(15)
C(8)-N(9)-N(10)	108.92(14)
N(10)-N(11)-N(12)	111.09(15)
N(11)-N(10)-N(9)	105.95(14)
C(8)-N(12)-N(11)	105.29(14)

Table S3. Hydrogen bonds for Compound **2** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1A)...N(3)#1	0.893(16)	2.080(16)	2.962(3)	170(2)
N(1)-H(1B)...N(4)#2	0.879(16)	2.117(16)	2.994(3)	175(2)
N(9)-H(9)...N(11)#3	0.88	1.99	2.851(3)	164.0

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

Table S4. Crystal data and structure refinement for Compound **4**.

Identification code	shrv475	
Empirical formula	$C_3H_4N_{10}O_2$	
Formula weight	212.16	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 15.6803(6) Å	α= 90°.
	b = 6.6171(3) Å	β= 115.8700(10)°.
	c = 17.0112(7) Å	γ = 90°.
Volume	1588.17(12) $Å^3$	
Z	8	
Density (-123°C)	1.775 Mg/m^3	
Density (20°C)	1.755 Mg/m^3	
Absorption coefficient	0.150 mm^{-1}	
F(000)	864	
Crystal size	0.283 x 0.162 x 0.074 mm^3	
Theta range for data collection	2.887 to 29.970°.	
Index ranges	-21<=h<=21, -9<=k<=7, -23<=l<=23	
Reflections collected	9002	
Independent reflections	2222 [R_{int} = 0.0165]	
Completeness to theta = 25.242°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7460 and 0.7083	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2222 / 0 / 136	
Goodness-of-fit on F^2	1.053	
Final R indices [I>2sigma(I)]	R_1 = 0.0336, wR_2 = 0.0863	
R indices (all data)	R_1 = 0.0385, wR_2 = 0.0899	
Largest diff. peak and hole	0.436 and -0.292 e.$Å^{-3}$	
CCDC No	1554454	

Table S5. Bond lengths [Å] and angles [°] for Compound **4**.

O(1)-N(3)	1.2380(12)	O(2)-N(3)	1.2413(12)
N(3)-N(4)	1.3520(11)	N(4)-C(5)	1.3382(13)
C(5)-N(6)	1.3493(13)	C(5)-N(9)	1.3514(12)
N(6)-N(7)	1.3704(12)	N(6)-H(6)	0.8800
N(7)-N(8)	1.2777(13)	N(8)-N(9)	1.3599(12)
N(9)-C(10)	1.4563(12)	C(10)-C(11)	1.4989(15)

C(10)-H(10A)	0.9900	C(10)-H(10B)	0.9900
C(11)-N(15)	1.3211(13)	C(11)-N(12)	1.3338(13)
N(12)-N(13)	1.3442(14)	N(12)-H(12)	0.8800
N(13)-N(14)	1.2930(13)	N(14)-N(15)	1.3636(13)
O(1)-N(3)-O(2)	122.37(9)	O(1)-N(3)-N(4)	122.19(9)
O(2)-N(3)-N(4)	115.43(8)	C(5)-N(4)-N(3)	114.78(8)
N(4)-C(5)-N(6)	136.96(9)	N(4)-C(5)-N(9)	119.23(9)
N(6)-C(5)-N(9)	103.80(8)	C(5)-N(6)-N(7)	109.58(8)
C(5)-N(6)-H(6)	125.2	N(7)-N(6)-H(6)	125.2
N(8)-N(7)-N(6)	108.42(9)	N(7)-N(8)-N(9)	107.75(8)
C(5)-N(9)-N(8)	110.45(8)	C(5)-N(9)-C(10)	127.37(8)
N(8)-N(9)-C(10)	122.18(8)	N(9)-C(10)-C(11)	110.39(8)
N(9)-C(10)-H(10A)	109.6	C(11)-C(10)-H(10A)	109.6
N(9)-C(10)-H(10B)	109.6	C(11)-C(10)-H(10B)	109.6
H(10A)-C(10)-H(10B)	108.1	N(15)-C(11)-N(12)	107.93(10)
N(15)-C(11)-C(10)	126.26(9)	N(12)-C(11)-C(10)	125.81(9)
C(11)-N(12)-N(13)	109.14(9)	C(11)-N(12)-H(12)	125.4
N(13)-N(12)-H(12)	125.4	N(14)-N(13)-N(12)	106.39(9)
N(13)-N(14)-N(15)	110.37(9)	C(11)-N(15)-N(14)	106.16(9)

Table S6. Hydrogen bonds for Compound **4** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(6)-H(6)...O(1)	0.88	2.15	2.5937(13)	110.4
N(6)-H(6)...N(15)#1	0.88	1.92	2.7603(12)	159.6
N(12)-H(12)...O(2)#2	0.88	2.44	3.0617(13)	128.2
N(12)-H(12)...O(2)#3	0.88	2.04	2.8614(12)	155.0

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

Table S7. Crystal data and structure refinement for Compound **10**.

Identification code	shrv431	
Empirical formula	$C_3H_{10}N_{12}O_2$	
Formula weight	246.23	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 5.8835(3) Å	α= 90°.
	b = 16.3726(7) Å	β= 98.4240(10)°.
	c = 10.5070(4) Å	γ = 90°.
Volume	1001.20(8) $Å^3$	
Z	4	
Density (-123°C)	1.634 Mg/m^3	
Denisty (20°C)	1.614 Mg/m^3	
Absorption coefficient	0.136 mm^{-1}	
F(000)	512	
Crystal size	0.421 x 0.339 x 0.259 mm^3	
Theta range for data collection	2.321 to 29.979°.	
Index ranges	-8<=h<=7, -21<=k<=22, -14<=l<=14	
Reflections collected	13803	
Independent reflections	2823 [R_{int} = 0.0167]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7460 and 0.7105	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2823 / 0 / 178	
Goodness-of-fit on F^2	1.052	
Final R indices [I>2sigma(I)]	R_1 = 0.0303, wR_2 = 0.0798	
R indices (all data)	R_1 = 0.0324, wR_2 = 0.0818	
Largest diff. peak and hole	0.404 and -0.270 $e.Å^{-3}$	
CCDC No	1554455	

Table S8. Bond lengths [Å] and angles [°] for Compound **10**.

O(1)-N(3)	1.2693(9)	O(2)-N(3)	1.2483(10)
N(3)-N(4)	1.3171(10)	N(4)-C(5)	1.3703(10)
C(5)-N(6)	1.3376(10)	C(5)-N(9)	1.3517(10)
N(6)-N(7)	1.3698(11)	N(7)-N(8)	1.2946(11)
N(8)-N(9)	1.3499(9)	N(9)-C(10)	1.4573(10)
C(10)-C(11)	1.4984(11)	C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900	C(11)-N(15)	1.3311(10)

C(11)-N(12)	1.3338(10)	N(12)-N(13)	1.3445(10)
N(13)-N(14)	1.3135(10)	N(14)-N(15)	1.3487(10)
N(16)-H(16B)	0.909(14)	N(16)-H(16D)	0.920(14)
N(16)-H(16C)	0.896(14)	N(16)-H(16A)	0.875(14)
N(17)-H(17A)	0.898(14)	N(17)-H(17B)	0.903(14)
N(17)-H(17D)	0.903(14)	N(17)-H(17C)	0.894(14)
O(2)-N(3)-O(1)	120.63(7)	O(2)-N(3)-N(4)	124.58(7)
O(1)-N(3)-N(4)	114.79(7)	N(3)-N(4)-C(5)	116.90(7)
N(6)-C(5)-N(9)	107.68(7)	N(6)-C(5)-N(4)	136.08(8)
N(9)-C(5)-N(4)	116.24(7)	C(5)-N(6)-N(7)	105.48(7)
N(8)-N(7)-N(6)	111.48(7)	N(7)-N(8)-N(9)	106.13(7)
N(8)-N(9)-C(5)	109.22(7)	N(8)-N(9)-C(10)	122.14(7)
C(5)-N(9)-C(10)	128.29(7)	N(9)-C(10)-C(11)	110.25(6)
N(9)-C(10)-H(10A)	109.6	C(11)-C(10)-H(10A)	109.6
N(9)-C(10)-H(10B)	109.6	C(11)-C(10)-H(10B)	109.6
H(10A)-C(10)-H(10B)	108.1	N(15)-C(11)-N(12)	111.99(7)
N(15)-C(11)-C(10)	124.86(7)	N(12)-C(11)-C(10)	123.13(7)
C(11)-N(12)-N(13)	104.60(7)	N(14)-N(13)-N(12)	109.50(7)
N(13)-N(14)-N(15)	109.35(7)	C(11)-N(15)-N(14)	104.56(7)
H(16B)-N(16)-H(16D)	110.7(12)	H(16B)-N(16)-H(16C)	107.6(12)
H(16D)-N(16)-H(16C)	107.4(12)	H(16B)-N(16)-H(16A)	110.8(12)
H(16D)-N(16)-H(16A)	109.2(12)	H(16C)-N(16)-H(16A)	111.1(12)
H(17A)-N(17)-H(17B)	109.2(12)	H(17A)-N(17)-H(17D)	113.6(12)
H(17B)-N(17)-H(17D)	104.8(12)	H(17A)-N(17)-H(17C)	107.4(12)
H(17B)-N(17)-H(17C)	110.7(12)	H(17D)-N(17)-H(17C)	111.1(12)

Table S9. Hydrogen bonds for Compound **10** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(16)-H(16B)...O(1)#1	0.909(14)	1.975(14)	2.8596(10)	163.9(12)
N(16)-H(16D)...N(12)#2	0.920(14)	1.995(14)	2.8926(10)	164.8(12)
N(16)-H(16C)...N(13)	0.896(14)	2.309(14)	3.0790(11)	144.0(12)
N(17)-H(17A)...O(1)#1	0.898(14)	2.086(15)	2.9693(11)	167.5(12)
N(17)-H(17B)...N(15)#1	0.903(14)	2.029(14)	2.9311(10)	177.5(12)
N(17)-H(17D)...N(14)#4	0.903(14)	2.109(14)	2.9865(11)	163.8(12)
N(17)-H(17C)...N(6)	0.894(14)	2.060(14)	2.9095(11)	158.3(12)
N(16)-H(16A)...N(13)#6	0.875(14)	2.172(14)	2.9794(11)	153.2(12)

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

Table S10. Crystal data and structure refinement for Compound **13**.

Identification code	shrv489	
Empirical formula	$C_9H_{16}N_{26}O_2$	
Formula weight	520.48	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 6.8412(2) Å	α= 90°.
	b = 16.3568(4) Å	β= 91.2720(10)°.
	c = 17.7892(4) Å	γ = 90°.
Volume	1990.12(9) $Å^3$	
Z	4	
Density (-123°C)	1.737 Mg/m^3	
Density (20°C)	1.717 Mg/m^3	
Absorption coefficient	0.138 mm^{-1}	
F(000)	1072	
Crystal size	0.354 x 0.220 x 0.105 mm^3	
Theta range for data collection	2.290 to 29.991°.	
Index ranges	-9<=h<=9, -22<=k<=20, -24<=l<=24	
Reflections collected	23403	
Independent reflections	5613 [R_{int} = 0.0240]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7460 and 0.7087	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5613 / 0 / 354	
Goodness-of-fit on F^2	1.026	
Final R indices [I>2sigma(I)]	R_1 = 0.0370, wR_2 = 0.0922	
R indices (all data)	R_1 = 0.0463, wR_2 = 0.0977	
Largest diff. peak and hole	0.300 and -0.337 $e.Å^{-3}$	
CCDC No	1554456	

Table S11. Bond lengths [Å] and angles [°] for Compound **13**.

O(1)-N(3)	1.2530(12)	O(2)-N(3)	1.2559(12)
N(3)-N(4)	1.3267(13)	N(4)-C(5)	1.3683(14)
C(5)-N(6)	1.3336(14)	C(5)-N(9)	1.3556(14)
N(6)-N(7)	1.3627(14)	N(7)-N(8)	1.2925(14)
N(8)-N(9)	1.3530(13)	N(9)-C(10)	1.4704(14)
C(10)-C(11)	1.4932(15)	C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900	C(11)-N(12)	1.3316(14)

C(11)-N(15)	1.3364(14)	N(12)-N(13)	1.3456(14)
N(13)-N(14)	1.3153(14)	N(14)-N(15)	1.3418(13)
N(16)-C(17)	1.3320(14)	N(16)-H(16A)	0.856(17)
N(16)-H(16B)	0.885(17)	C(17)-N(26)	1.3434(14)
C(17)-N(18)	1.3482(14)	N(18)-C(24)	1.3535(14)
N(18)-N(19)	1.3960(12)	N(19)-C(20)	1.3185(15)
C(20)-N(21)	1.3352(14)	C(20)-N(22)	1.3975(14)
N(21)-H(21A)	0.8800	N(21)-H(21B)	0.8800
N(22)-C(24)	1.3629(14)	N(22)-N(23)	1.3936(13)
N(23)-H(23A)	0.872(19)	N(23)-H(23B)	0.915(19)
C(24)-N(25)	1.3117(14)	N(25)-N(26)	1.4087(13)
N(26)-H(26)	0.8800	N(27)-C(28)	1.3219(14)
N(27)-H(27A)	0.8800	N(27)-H(27B)	0.8800
C(28)-N(37)	1.3418(14)	C(28)-N(29)	1.3461(13)
N(29)-C(35)	1.3602(13)	N(29)-N(30)	1.3965(12)
N(30)-C(31)	1.3301(14)	C(31)-N(32)	1.3237(14)
C(31)-N(33)	1.3958(14)	N(32)-H(32A)	0.8800
N(32)-H(32B)	0.8800	N(33)-C(35)	1.3694(14)
N(33)-N(34)	1.3976(13)	N(34)-H(34A)	0.899(16)
N(34)-H(34B)	0.867(16)	C(35)-N(36)	1.3055(14)
N(36)-N(37)	1.4112(13)	N(37)-H(37)	0.8800

O(1)-N(3)-O(2)	120.15(9)	O(1)-N(3)-N(4)	115.62(9)
O(2)-N(3)-N(4)	124.23(9)	N(3)-N(4)-C(5)	115.77(9)
N(6)-C(5)-N(9)	107.97(9)	N(6)-C(5)-N(4)	134.25(10)
N(9)-C(5)-N(4)	117.77(9)	C(5)-N(6)-N(7)	105.35(9)
N(8)-N(7)-N(6)	111.95(9)	N(7)-N(8)-N(9)	106.00(9)
N(8)-N(9)-C(5)	108.68(9)	N(8)-N(9)-C(10)	122.35(9)
C(5)-N(9)-C(10)	128.26(9)	N(9)-C(10)-C(11)	111.28(9)
N(9)-C(10)-H(10A)	109.4	C(11)-C(10)-H(10A)	109.4
N(9)-C(10)-H(10B)	109.4	C(11)-C(10)-H(10B)	109.4
H(10A)-C(10)-H(10B)	108.0	N(12)-C(11)-N(15)	112.25(10)
N(12)-C(11)-C(10)	125.05(10)	N(15)-C(11)-C(10)	122.70(10)
C(11)-N(12)-N(13)	104.33(9)	N(14)-N(13)-N(12)	109.48(9)
N(13)-N(14)-N(15)	109.65(9)	C(11)-N(15)-N(14)	104.28(9)
C(17)-N(16)-H(16A)	118.3(11)	C(17)-N(16)-H(16B)	115.8(10)
H(16A)-N(16)-H(16B)	116.9(14)	N(16)-C(17)-N(26)	130.64(10)
N(16)-C(17)-N(18)	125.05(10)	N(26)-C(17)-N(18)	104.28(9)
C(17)-N(18)-C(24)	107.87(9)	C(17)-N(18)-N(19)	137.64(9)
C(24)-N(18)-N(19)	114.21(9)	C(20)-N(19)-N(18)	101.00(9)
N(19)-C(20)-N(21)	125.79(11)	N(19)-C(20)-N(22)	113.92(9)
N(21)-C(20)-N(22)	120.24(11)	C(20)-N(21)-H(21A)	120.0
C(20)-N(21)-H(21B)	120.0	H(21A)-N(21)-H(21B)	120.0
C(24)-N(22)-N(23)	130.59(9)	C(24)-N(22)-C(20)	105.94(9)
N(23)-N(22)-C(20)	123.04(9)	N(22)-N(23)-H(23A)	108.1(12)
N(22)-N(23)-H(23B)	108.0(11)	H(23A)-N(23)-H(23B)	111.0(16)

N(25)-C(24)-N(18)	113.84(10)	N(25)-C(24)-N(22)	141.21(10)
N(18)-C(24)-N(22)	104.90(9)	C(24)-N(25)-N(26)	100.69(9)
C(17)-N(26)-N(25)	113.30(9)	C(17)-N(26)-H(26)	123.4
N(25)-N(26)-H(26)	123.4	C(28)-N(27)-H(27A)	120.0
C(28)-N(27)-H(27B)	120.0	H(27A)-N(27)-H(27B)	120.0
N(27)-C(28)-N(37)	129.11(10)	N(27)-C(28)-N(29)	126.44(10)
N(37)-C(28)-N(29)	104.42(9)	C(28)-N(29)-C(35)	107.51(9)
C(28)-N(29)-N(30)	137.82(9)	C(35)-N(29)-N(30)	114.48(9)
C(31)-N(30)-N(29)	100.88(8)	N(32)-C(31)-N(30)	126.26(10)
N(32)-C(31)-N(33)	119.92(10)	N(30)-C(31)-N(33)	113.80(9)
C(31)-N(32)-H(32A)	120.0	C(31)-N(32)-H(32B)	120.0
H(32A)-N(32)-H(32B)	120.0	C(35)-N(33)-C(31)	106.27(9)
C(35)-N(33)-N(34)	131.45(9)	C(31)-N(33)-N(34)	122.27(9)
N(33)-N(34)-H(34A)	109.9(10)	N(33)-N(34)-H(34B)	109.3(10)
H(34A)-N(34)-H(34B)	109.9(14)	N(36)-C(35)-N(29)	114.17(10)
N(36)-C(35)-N(33)	141.18(10)	N(29)-C(35)-N(33)	104.56(9)
C(35)-N(36)-N(37)	100.48(8)	C(28)-N(37)-N(36)	113.42(9)
C(28)-N(37)-H(37)	123.3	N(36)-N(37)-H(37)	123.3

Table S12. Hydrogen bonds for Compound **13** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(16)-H(16A)...N(7)#1	0.856(17)	2.096(17)	2.9361(15)	166.9(15)
N(16)-H(16B)...N(14)#2	0.885(17)	2.014(17)	2.8744(14)	163.6(14)
N(21)-H(21A)...N(12)#3	0.88	2.35	3.0078(14)	131.4
N(21)-H(21B)...N(8)#3	0.88	2.39	3.1532(15)	144.7
N(23)-H(23A)...N(15)#4	0.872(19)	2.157(19)	3.0168(15)	168.9(16)
N(26)-H(26)...O(2)#1	0.88	2.24	2.9778(13)	140.6
N(26)-H(26)...N(6)#1	0.88	2.11	2.8784(13)	145.1
N(27)-H(27A)...O(1)#6	0.88	2.31	2.9247(13)	126.6
N(27)-H(27A)...O(2)#6	0.88	2.06	2.9355(13)	174.1
N(27)-H(27B)...N(15)#7	0.88	2.23	3.0403(14)	152.6
N(32)-H(32A)...O(1)#7	0.88	2.11	2.8623(13)	143.2
N(32)-H(32B)...N(13)#3	0.88	2.19	2.9604(14)	146.7
N(34)-H(34A)...N(12)	0.899(16)	2.277(16)	3.1624(15)	168.6(14)
N(37)-H(37)...N(25)#8	0.88	2.09	2.9488(13)	163.8

Symmetry transformations used to generate equivalent atoms:
#1 -x+3/2,y-1/2,-z+3/2 #2 x-1,y,z #3 -x+2,-y+2,-z+1
#4 x-1/2,-y+3/2,z-1/2 #5 x+1/2,-y+3/2,z-1/2
#6 -x+1,-y+2,-z+2 #7 -x+3/2,y+1/2,-z+3/2 #8 x-1/2,-y+3/2,z+1/2

Table S13 Energetic properties of compounds **2** **13**

	ρ[a]	Dv[b]	P[c]	ΔH_f[d]	T_m[e]	T_{dec}[f]	IS[g]	FS[h]	N[i]	$N+O$[j]
	(g·cm^3)	(m/s)	(GPa)	(kJ/g)	(°C)	(°C)	(J)	(N)	(%)	(%)
2	1.61	7780	20.9	3.20	213	217	>40	>360	75.43	75.43
3	1.79	8857	31.2	1.95	147	156	28	240	60.86	81.71
4	1.76	8652	29.6	2.90	_	178	12	160	66.03	81.11
5	1.49	7476	18.1	2.74	172	239	>40	>360	76.06	76.06
6	1.60	8330	23.5	3.26	150	244	>40	>360	77.36	77.36
7	1.59	8155	23.1	2.75	164	172	>40	>360	69.98	77.97
8	1.62	7912	21.5	3.20	241	246	>40	>360	74.12	74.12
9	1.94	7174	19.3	0.41	_	306	>40	>360	48.58	59.68
10	1.60	8076	22.6	1.57	_	229	>40	>360	68.27	81.27
11	1.62	8654	26.9	2.64	_	224	>40	>360	70.99	82.57
12	1.69	8778	29.5	1.83	_	186	>40	>360	60.42	83.42
13	1.71	8499	26.5	3.14	147	238	>40	>360	69.98	76.13
TNT	1.65	7303	21.3	-0.26	81	295	15	>353	18.50	60.76
RDX	1.80	8795	34.9	0.32	_	204	7.5	120	37.84	81.06

[a] Density - gas pycnometer at 25 °C; [b] Calculated detonation velocity; [c] Calculated detonation pressure; [d] Calculated molar enthalpy of formation; [e] Melting point (onset); [f] Temperature of decomposition (onset); [g] Impact sensitivity; [h] Friction sensitivity; [i] Nitrogen content; [j] Combined nitrogen and oxygen content.