Sandwich-like Low-sensitive Nitroamine Explosives Stabilized by Hydrogen Bonds and π-π Stacking Interactions

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1. Table S1 Crystal data and structure refinement for 2a and 4b

Identification code	**2a**	**4b**
Empirical formula	$C_9H_{13}N_{13}O_6$	$C_{16}H_{29}N_{30}O_{12}$
Formula weight	399.29	825.69
Temperature/K	150.0 (2)	150.0 (2)
Crystal system	Triclinic	monoclinic
Space group	P-1	$P2_1/c$
a/Å	8.677(2)	21.16(5)
b/Å	9.036(4)	13.182(9)
c/Å	10.283(4)	11.89(2)
α/°	77.57(3)	90
β/°	78.49(3)	105.45(18)
γ/°	78.960(19)	90
Volume/Å^3	762.2(5)	3196(10)
Z	2	4
ρ_{calc}g/cm^3	1.74	1.72
μ/mm^{-1}	0.821	0.812
F(000)	413.3	1708
Crystal size/mm^3	0.26 × 0.22 × 0.15	0.18 × 0.16 × 0.1
Radiation	GaKα (λ = 1.34138)	GaKα (λ = 1.34138)
2Θ range for data collection/°	7.76 to 109.82	6.946 to 110.042
Index ranges	-10≤h≤10, -11≤k≤11,-12≤l≤12	-24≤h≤25, -14≤k≤16, -14≤l≤14
Reflections collected	10801	18886
Independent reflections	2891 [R_{int} = 0.0329, R_{sigma} = 0.0280]	5793 [R_{int} = 0.0470, R_{sigma} = 0.0491]

Data/restraints/parameters	2891/7/265	5793/33/559
Goodness-of-fit on F^2	1.07	1.043
Final R indexes [I>=2σ (I)]	$R_1 = 0.0391$, $wR_2 = 0.0990$	$R_1 = 0.0769$, $wR_2 = 0.2011$
Final R indexes [all data]	$R_1 = 0.0448$, $wR_2 = 0.1044$	$R_1 = 0.1039$, $wR_2 = 0.2248$
Largest diff. peak and hole	0.50 and -0.31 e.Å^{-3}	0.48 and -0.72 e.Å^{-3}

2. Selected bond lengths, bond angles for 2a.

Table S2. Bond lengths [Å] for 2a

Atom-atom	Length/Å	Atom-atom	Length/Å
O(4))-N(1)	1.252(2)	N(7)-C(17)	1.358(2)
O(7)-N(4)	1.249(2)	N(10)-N(11)	1.377(2)
O(6)-N(4)	1.241(2)	N(10)-N(18)	1.326(2)
O(5)-N(1)	1.254(2)	N(11)-C(16)	1.306(2)
N(6)-N(5)	1.404(2)	N(2)-N(1)	1.332(2)
N(6)-C(16)	1.390(2)	N(4)-N(5)	1.346(2)
N(6)-N(18)	1.359(2)	N(8)-C(17)	1.319(2)
N(13)-N(12)	1.379(2)	N(9)-C(18)	1.319(2)
N(13)-C(17)	1.328(2)	C(10)-C(16)	1.474(2)
N(3)-C(10)	1.342(2)	C(10)-C(11)	1.391(2)
N(3)-C(14)	1.339(2)	C(15)-C(14)	1.475(2)
N(12)-C(15)	1.300(2)	C(14)-C(13)	1.393(2)
N(7)-N(2)	1.411(2)	C(11)-C(12)	1.387(2)
N(7)-C(15)	1.388(2)	C(13)-C(12)	1.386(2)

Table S3. Bond angles [°] for 2a.

Atom-atom-atom	Angle/	Atom-atom-atom	Angle/
C(16)-N(6)-N(5)	130.85(14)	C(11)-C(10)-N(3)	123.64(15)
C(18)-N(6)-N(5)	122.20(14)	C(11)-C(10)-C(16)	123.17(15)
C(18)-N(6)-C(16)	106.96(14)	N(7)-C(15)-N(12)	110.89(15)
C(17)-N(12)-N(12)	111.97(14)	C(14)-C(15)-N(7)	126.28(15)
C(14)-N(3)-C(10)	117.07(14)	N(11)-C(16)-N(6)	110.42(14)
C(15)-N(12)-N(13)	104.58(14)	C(10)-C(16)-N(6)	126.62(15)
C(15)-N(7)-N(2)	128.27(14)	C(10)-C(16)-N(11)	122.95(15)
C(17)-N(7)-N(3)	123.40(14)	C(15)-C(14)-N(3)	113.56(14)
C(17)-N(7)-C(15)	106.73(14)	C(13)-C(14)-N(3)	123.75(15)
C(18)-N(10)-N(11)	112.14(14)	C(13)-C(14)-C(15)	122.60(15)
C(16)-N(11)-N(10)	104.73(14)	C(12)-C(11)-C(10)	118.04(15)
N(1)-N(2)-N(7)	108.84(13)	C(12)-C(13)-C(14)	117.94(15)
O(5)-N(1)-O(4)	120.99(15)	N(10)-C(18)-N(6)	105.75(14)

N(2)-N(1)-O(4)	115.66(15)	N(9)-C(18)-N(6)	125.93(16)
N(2)-N(1)-O(5)	123.34(14)	N(9)-C(18)-N(10)	128.32(16)
O(6)-N(4)-O(7)	122.02(16)	C(13)-C(12)-C(11)	119.52(15)
N(5)-N(4)-O(7)	123.09(14)	N(7)-C(17)-N(13)	105.79(15)
N(5)-N(4)-O(6)	114.87(15)	N(8)-C(17)-N(13)	127.48(16)
N(4)-N(5)-N(6)	109.31(13)	N(8)-C(17)-N(7)	126.69(17)
C(16)-C(10)-N(3)	113.15(14)		

Table S4 Hydrogen bonds present in 2a

D−H···A	d(D−H) /Å	d(H−A) /Å	d(D−A)/Å	D−H−A /°
N3−H3···O5	0.88	1.87(7)	2.69(4)	153(6)
N9−H9···O3^{i}	0.88	2.26(8)	2.86(3)	124(7)
N9−H9···O1^{ii}	0.88	2.22(5)	2.95(3)	139(8)
N4−H4A···N12^{iii}	0.88	2.13(1)	3.00	169(2)
N4−H4B···O6^{iv}	0.88	2.00(7)	2.83(9)	157(3)
N10−H10A···O1^{ii}	0.88	2.34(2)	3.06(3)	139(2)
N10−H10B···O5^{v}	0.88	2.12(4)	2.93(6)	153(1)
C3−H3A···O4^{vi}	0.95	2.51(3)	3.09(4)	119(5)
C3−H3A···N12	0.95	2.46(2)	3.09(7)	124(1)
C5−H5···O1	0.95	2.63(5)	3.44(2)	142(9)
C5−H5A···N1	0.95	2.59(4)	3.37(2)	139(3)
O5−H5A···O6	0.99(6)	1.74(4)	2.73(9)	177(5)
O5−H5B···O2^{vii}	0.71(8)	2.57(4)	2.90(4)	110(4)
O5−H5B···O5^{viii}	0.71(8)	2.33(6)	2.85(2)	130(1)

Symmetry codes: (i) -x+2, -y+1, -z; (ii) x+1, y, z-1; (iii) x, y-1, z+1; (iv) x-1, y, z; (v) x, y+1, z-1 ; (vi) -x+1, -y+2, -z; (vii) x+1, y, z; (viii) -x+2, -y, -z+1.

Table S5. Bond lengths [Å] for 4b.

Atom-atom	Length/Å	Atom-atom	Length/Å
O(1)-N(8)	1.257(4)	N(11)-C(9)	1.299(6)
O(2)-N(8)	1.256(5)	N(9)-N(10)	1.386(5)
O(8)-N(22)	1.245(5)	N(9)-C(8)	1.309(5)
O(6)-N(28)	1.256(4)	N(10)-C(9)	1.350(6)
O(3)-N(14)	1.242(4)	N(6)-N(7)	1.414(6)
O(4)-N(14)	1.266(5)	N(6)-C(6)	1.375(6)
O(5)-N(28)	1.256(5)	N(6)-C(7)	1.370(5)
O(7)-N(22)	1.243(4)	N(7)-N(8)	1.325(4)
N(17)-N(18)	1.385(5)	N(5)-C(7)	1.323(6)
N(17)-C(14)	1.313(5)	N(4)-N(3)	1.395(5)
N(8)-C(15)	1.326(6)	N(4)-C(7)	1.326(6)

N(20)-N(21)	1.391(5)	N(3)-C(6)	1.311(5)
N(20)-C(15)	1.363(5)	N(16)-C(11)	1.335(5)
N(13)-N(14)	1.339(4)	C(13)-C(12)	1.393(6)
N(20)-C(14)	1.386(6)	N(16)-C(12)	1.342(5)
N(21)-N(22)	1.341(4)	N(15)-C(13)	1.340(5)
N(9)-C(15)	1.334(6)	N(15)-C(10)	1.339(5)
N(26)-N(27)	1.401(5)	N(2)-C(4)	1.343(6)
N(26)-C(16)	1.389(6)	N(2)-C(3)	1.329(5)
N(26)-C(17)	1.376(5)	N(1)-C(2)	1.339(5)
N(27)-N(28)	1.332(4)	N(1)-C(5)	1.331(5)
N(25)-C(17)	1.328(6)	C(11)-C(14)	1.466(6)
N(23)-N(24)	1.395(5)	C(11)-C(10)	1.401(6)
N(23)-C(16)	1.298(5)	C(6)-C(2)	1.466(6)
N(24)-C(17)	1.321(6)	C(4)-C(8)	1.466(5)
N(12)-N(13)	1.400(5)	C(4)-C(5)	1.388(6)
N(12)-C(9)	1.364(5)	C(16)-C(13)	1.465(5)
N(12)-C(8)	1.380(6)	C(2)-C(3)	1.392(6)

Table S6. Bond angles [°] for 4b.

Atom-atom-atom	Angle/	Atom-atom-atom	Angle/
C(14)-N(17)-N(17)	105.3(3)	N(16)-C(11)-C(14)	119.5(4)
C(15)-N(18)-N(17)	110.9(3)	N(16)-C(11)-C(10)	121.4(4)
C(15)-N(20)-N(21)	123.9(3)	C(10)-C(11)-C(14)	119.1(4)
C(15)-N(20)-C(14)	106.5(3)	N(18)-C(15)-N(20)	106.9(3)
C(14)-N(20)-N(21)	129.2(3)	N(18)-C(15)-N(19)	128.1(4)
N(22)-N(21)-N(20)	109.3(3)	N(19)-C(15)-N(20)	125.0(4)
O(8)-N(22)-N(21)	114.8(3)	N(6)-C(6)-C(2)	127.5(3)
O(7)-N(22)-O(8)	122.0(3)	N(3)-C(6)-N(6)	109.8(3)
O(7)-N(22)-N(21)	123.2(3)	N(3)-C(6)-C(2)	122.7(4)
C(16)-N(26)-N(27)	131.0(3)	N(5)-C(7)-N(6)	122.5(4)
C(17)-N(26)-N(27)	122.6(3)	N(5)-C(7)-N(4)	128.5(3)
C(17)-N(26)-C(16)	106.0(3)	N(4)-C(7)-N(6)	108.9(4)
N(28)-N(27)-N(26)	108.7(3)	N(2)-C(4)-C(8)	119.0(4)
O(6)-N(28)-N(27)	123.6(3)	N(2)-C(4)-C(5)	121.5(4)
O(5)-N(28)-O(6)	121.0(3)	C(5)-C(4)-C(8)	119.5(4)
O(5)-N(28)-N(27)	115.3(3)	N(17)-C(14)-N(20)	110.4(3)
C(16)-N(23)-N(24)	106.6(3)	N(17)-C(14)-C(11)	121.7(4)
C(17)-N(24)-N(23)	109.5(3)	N(20)-C(14)-C(11)	127.9(4)
C(9)-N(12)-N(13)	122.5(3)	N(11)-C(9)-N(12)	125.2(4)
C(9)-N(12)-C(8)	107.0(3)	N(11)-C(9)-N(10)	128.4(3)
C(8)-N(12)-N(13)	130.1(3)	N(10)-C(9)-N(12)	106.4(4)
N(14)-N(13)-N(12)	108.3(3)	N(26)-C(16)-C(13)	127.3(4)
O(3)-N(14)-O(4)	121.7(3)	N(23)-C(16)-N(26)	110.2(3)

O(3)-N(14)-N(13)	124.3(3)	N(23)-C(16)-C(13)	122.5(4)
O(4)-N(14)-N(13)	114.0(3)	N(12)-C(8)-C(4)	127.5(3)
C(8)-N(9)-N(10)	105.7(3)	N(9)-C(8)-N(12)	110.7(3)
C(9)-N(10)-N(9)	110.2(3)	N(9)-C(8)-C(4)	121.8(4)
C(6)-N(6)-N(7)	131.3(3)	N(25)-C(17)-N(26)	123.7(4)
C(7)-N(6)-N(7)	122.5(3)	N(24)-C(17)-N(26)	107.6(3)
C(7)-N(6)-C(6)	106.0(3)	N(24)-C(17)-N(25)	128.6(3)
N(8)-N(7)-N(6)	108.9(3)	N(1)-C(2)-C(6)	118.9(4)
O(1)-N(8)-N(7)	123.6(3)	N(1)-C(2)-C(3)	122.3(4)
O(2)-N(8)-O(1)	121.0(3)	C(3)-C(2)-C(6)	118.9(3)
O(2)-N(8)-N(7)	115.4(3)	N(15)-C(13)-C(16)	119.5(4)
C(7)-N(4)-N(3)	107.8(3)	N(15)-C(13)-C(12)	121.6(4)
C(6)-N(3)-N(4)	107.4(3)	C(12)-C(13)-C(16)	118.9(4)
C(11)-N(16)-C(12)	116.4(4)	N(15)-C(10)-C(11)	122.2(4)
C(10)-N(15)-C(13)	116.2(4)	N(16)-C(10)-C(11)	122.2(4)
C(3)-N(2)-C(4)	116.4(4)	N(2)-C(3)-C(2)	121.6(4)
C(5)-N(1)-C(2)	115.7(4)	N(1)-C(5)-C(4)	122.5(4)

Table S7 Hydrogen bonds present in 4b

D−H···A	d(D−H) /Å	d(H−A) /Å	d(D−A)/Å	D−H−A /°
N18−H18···N23^{i}	0.88	2.65(6)	3.51(4)	165(2)
N18−H18···N24^{i}	0.88	1.83(8)	2.69(4)	163(8)
N19−H19A···O7^{ii}	0.88	2.40(4)	3.20(1)	150(7)
N19−H19A···O9^{iii}	0.88	2.08(3)	2.74(2)	131(0)
N19−H19B···O4^{iv}	0.88	2.13(3)	2.90(7)	146(5)
N25−H25A···O6^{v}	0.88	2.25	3.02	145(9)
N25−H25B···O2^{vi}	0.88	2.13(5)	2.90(6)	145(9)
N11−H11A···O3^{vii}	0.88	2.35(6)	3.17(9)	155(8)
N11−H11A···O12^{viii}	0.88	2.22(8)	2.85	127(4)
N11−H11B···O8^{ix}	0.88	2.28(6)	3.01(5)	140(1)
N5−H5A···O1^{x}	0.88	2.20(2)	2.98(4)	147(7)
N5−H5B···O5^{xi}	0.88	2.39(2)	3.08(5)	135(8)
N4−H4···N9^{i}	0.88	2.67(1)	3.54	169(6)
N4−H4···N10^{i}	0.88	1.96(9)	2.80(4)	157(9)
N30−H30A···N7^{vi}	0.96(8)	1.96(9)	2.89(2)	158(6)
N30−H30B···N13	0.96	2.53(2)	3.04(1)	113(2)
N30−H30B···N2	0.96	2.34(4)	3.12(9)	138(4)
N30−H30C···N21^{iv}	0.96(8)	2.07	3.00(8)	162(6)

N30−H30D···O11	0.99(4)	1.74(5)	2.73(9)	178(9)
C10−H10···O6^{ii}	0.95	2.57(3)	3.49(6)	164
C10−H10···O9	0.95	2.55(6)	3.16(9)	122(5)
C12−H12···O7^{v}	0.95	2.49(5)	3.39(2)	157(6)
C3−H3···O3^{x}	0.95	2.53	3.43(6)	159(6)
C5−H5···O1^{vii}	0.95	2.63(8)	3.55(9)	163(5)
N29−H29A···O10	0.95(1)	2.22(8)	2.78	116(1)
N29−H29B···N21^{iv}	0.963	2.61(6)	3.31(2)	129(4)
N29−H29B···N16^{iv}	0.963	2.1(8)	3.07(2)	153(4)
N29−H29C···O11	0.959	1.87(6)	2.80(3)	161(5)
N29−H29D···O4^{x}	0.96(1)	1.98(8)	2.94	170(2)
N29−H29D···N14^{x}	0.96(1)	2.65(2)	3.50(5)	148(1)

Symmetry codes: (i) x, y, z-1; (ii) x, -y+1/2, z-1/2; (iii) -x+1, -y+1, -z; (iv) -x+1, -y+1, -z+1; (v) x, -y+1/2, z+1/2 ; (vi)-x+2, -y+1, -z+2; (vii)x, -y+3/2, z+1/2; (viii) x, y, z+1; (xi)-x+1, y+1/2, -z+3/2; (x) x, -y+3/2, z-1/2; (xi) -x+2, y+1/2, -z+3/2;

3. Computational details.

All calculations were carried out using the Gaussian G16 (revision C.01) program package, The enthalpies (H) were calculated using the modified CBS-4M method. The enthalpies of the gasphase species M were computed according to the atomization energy method [Equation (1)]. The results obtained from theoretical calculations at the CBS-4M level of theory were given in Table 3. The calculated enthalpy of cations and the enthalpy of formation of the atom were obtained from reference 1 and NIST WebBook. Meanwhile, the solid-phase heat of formation is calculated on the basis of Born-Haber energy cycle [Equation (1)][2].

$$\Delta_f H^\circ_{(g,M,298)} = H_{(molecule,298)} - \sum H^\circ_{(Atoms,298)} + \sum \Delta_f H^\circ_{(Atoms,298)} \quad (1)$$

$$\Delta H_{sub} = 188 \times T_m \quad (2)$$

T_m represents the melting point or decomposition temperature of a substance

Table S8. Results obtained from theoretical calculations at the CBS-4M level of theory.

	−H / a.u.
2a	1358.928877
2a$^-$	1357.883768
2b	1374.955214
2b$^-$	1373.916249
NH_4^+	56.796608
NH_3OH^+	131.211668
AG^+	260.701802

Table 7. Literature values for atomic ΔH_f^{298} /kcal·mol^{-1}.

	−H / a.u.	NIST/ kcal·mol^{-1}
C	37.786156	171.3
H	0.500991	52.1
N	54.522462	113
O	74.991202	59.6

4. Detonation Products predicted by EXPLO5

2a				2b			
Detonation Products	mol/mol	mol/kg	Mol %	Detonation Products	mol/mol	mol/kg	Mol %
C(d)	8.166756E00	2.248172E01	46.2680	C(d)	7.071049E00	1.941252E01	39.1213
N_2	6.229522E00	1.714884E01	33.0044	N_2	6.792320E00	1.864731E01	37.5792
H_2O	2.976388E00	8.193501E00	15.7691	H_2O	2.756539E00	7.567669E00	15.2508
NH_3	5.210898E-01	1.434474E00	2.7608	NH_3	3.958402E-01	1.086721E00	2.1900
CO	2.741711E-01	7.547477E-1	1.4526	CO	3.446338E-01	9.461410E-01	1.9067
CH_2O_2	2.607833E-01	7.178930E-01	1.3816	CH_2O_2	2.833581E-01	7.779178E-01	0.9176
H_2	1.771826E-01	4.877544E-01	0.9387	CO_2	1.658511E-01	4.553196E-01	0.8240
CO_2	1.136998E-01	3.129966E-01	0.6024	H_2	1.489337E-01	4.088754E-01	0.4266
CH_4	1.052564E-01	2.897534E-01	0.5577	CH_4	7.710529E-02	2.116812E-01	0.1048
C_2H_6	2.231724E-02	6.143565E-02	0.1182	HCN	1.893501E-02	5.198327E-02	0.0756
HCN	1.900873E-02	5.232789E-02	0.1007	C_2H_6	1.365628E-02	3.749130E-02	0.0314
C_2H_4	7.607564E-03	2.094236E-02	0.0403	C_2H_4	5.672969E-03	1.557430E-02	0.0022
CH_3OH	4.658569E-04	1.282427E-03	0.0025	CH_3OH	3.977811E-04	1.092049E-03	0.0014
N_2H_4	3.738742E-04	1.029214E-03	0.0020	N_2H_4	2.464372E-04	6.765569E-04	0.0005
NH_2	1.066458E-04	2.935783E-04	0.0006	NH_2	8.873934E-05	2.436207E-04	0.0003
H	6.899877E-05	1.899422E-04	0.0004	H	6.104165E-05	1.675808E-04	0.0000
CH_2O	6.406353E-06	1.763563E-05	0.0000	CH_2O	7.420622E-06	2.037222E-05	0.0000
CHNO	1.545425E-06	4.254298E-06	0.0000	CHNO	2.126826E-06	5.838887E-06	0.0000
CNO	1.345320E-06	3.703443E-06	0.0000	CNO	1.608100E-06	4.414801E-06	0.0000
N	2.213128E-07	6.092375E-07	0.0000	N	1.944616E-07	5.338656E-07	0.0000
N_2O	1.954458E-08	5.380299E-08	0.0000	N_2O	2.454710E-08	6.739004E-08	0.0000
NO_2	6.125567E-09	1.686267E-08	0.0000	NO_2	7.334994E-09	2.013714E-08	0.0000
C(gr)	5.075377E-10	1.397167E-09	0.0000	C(gr)	5.728141E-10	1.572576E-09	0.0000

3a				3b			
Detonation Products	mol/mol	mol/kg	Mol %	Detonation Products	mol/mol	mol/kg	Mol %
C(d)	8.151796E00	1.889877E01	36.0811	C(d)	7.367112E00	1.704048E01	33.7499
N_2	6.793532E00	1.574983E01	30.0692	N_2	7.103334E00	1.643035E01	32.5415
H_2O	5.189306E00	1.203066E01	22.9687	H_2O	5.004043E00	1.157459E01	22.9243
NH_3	1.391270E00	3.228010E00	6.1628	NH_3	1.238155E00	2.863912E00	5.6722
CH_2O_2	2.921644E-01	6.773413E-01	1.2932	CH_2O_2	3.500020E01	8.095714E-01	1.6034
H_2	2.908092E-01	6.741995E-01	0.9144	H_2	2.769351E-01	6.405651E-01	1.2687

CH_4	2.065993E-01	4.789708E-01	0.6107	CO	1.828211E-01	4.228739E-01	0.8375
CO	1.379805E-01	3.198880E-01	0.2788	CH_4	1.634098E-01	3.779747E-01	0.7486
C_2H_6	6.299876E-02	1.460536E-01	0.1944	CO_2	5.627539E-02	1.301677E-01	0.2578
CO_2	4.392691E-02	1.018382E-01	0.0758	C_2H_6	4.774081E-02	1.104268E-01	0.2187
HCN	1.713435E-02	3.972354E-02	0.0528	HCN	2.346110E-02	5.426665E-02	0.1075
C_2H_4	1.193483E-02	2.766920E-02	0.0072	C_2H_4	1.231668E-02	2.848907E-02	0.0564
N_2H_4	1.627335E-03	3.772473E-03	0.0023	N_2H_4	1.950773E-03	4.512232E-03	0.0089
CH_3OH	5.280011E-04	1.224095E-03	0.0008	CH_3OH	5.755738E-04	1.331330E-03	0.0026
NH_2	1.745855E-04	4.047514E-04	0.0004	NH_2	2.542645E-04	5.881260E-04	0.0012
H	9.314290E-05	2.159385E-04	0.0000	H	1.415727E-04	3.274644E-04	0.0006
CH_2O	1.956109E-06	4.534959E-06	0.0000	CH_2O	2.908948E-06	6.728535E-06	0.0000
CHNO	7.796956E-07	1.807613E-06	0.0000	CNO	1.887113E-06	4.364983E-06	0.0000
CNO	4.576433E-07	1.060980E-06	0.0000	N	1.112726E-06	2.573788E-06	0.0000
N	2.692463E-07	6.242091E-07	0.0000	CHNO	4.723254E-07	1.092511E-06	0.0000
N_2O	9.583186E-09	2.221724E-08	0.0000	N_2O	2.264355E-08	5.237560E-08	0.0000
NO_2	5.813614E-09	1.347803E-08	0.0000	NO_2	1.664178E-08	3.849324E-08	0.0000
C(gr)	2.593515E-10	6.012693E-10	0.0000	C(gr)	2.701193E-10	6.247989E-10	0.0000

4a				**4b**			
Detonation Products	mol/mol	mol/kg	Mol %	Detonation Products	mol/mol	mol/kg	Mol %
C(d)	8.098136E00	2.027870E01	37.9683	C(d)	7.220937E00	1.803737E01	34.7815
N_2	6.477502E00	1.622044E01	30.3699	N_2	7.052676E00	1.761707E01	33.9710
H_2O	3.769883E00	9.440236E00	17.6752	H_2O	3.735013E00	9.329790E00	17.9907
NH_3	2.040287E00	5.109121E00	9.5659	NH_3	1.888233E00	43746667E00	5.0952
CH_4	4.233688E-01	1.060166E00	1.9850	CH_4	3.517244E-01	8.785818E-01	1.6942
H_2	2.139862E-01	5.358471E-01	1.0033	H_2	2.205531E-01	5.509256E-01	1.0624
C_2H_6	1.669886E-01	4.181592E-01	0.7829	C_2H_6	1.292613E-01	3.228853E-01	0.6226
CH_2O_2	9.113134E-02	2.282037E-01	0.4273	CH_2O_2	1.018808E-01	2.544907E-01	0.4907
CO	2.531349E-02	6.338800E-02	0.1187	CO	3.405826E-02	8.507504E-02	0.1641
CO_2	1.115938E-02	2.794443E-02	0.0523	CO_2	1.346249E-02	3.362832E-02	0.0648
C_2H_4	6.686028E-03	1.674261E-02	0.0313	C_2H_4	7.218053E-03	1.803016E-02	0.0348
HCN	3.320007E-03	8.313692E-03	0.0156	HCN	4.736482E-03	1.183139E-02	0.0228
N_2H_4	6.839922E-04	1.712798E-03	0.0032	N_2H_4	8.241594E-04	2.028690E-03	0.0040
CH_3OH	2.218795E-04	5.556127E-04	0.0010	CH_3OH	2.413067E-04	6.027665E-04	0.0012
NH_2	1.932234E-05	4.838543E-05	0.0001	NH_2	3.007431E-05	7.512343E-05	0.0001
H	5.856217E-06	1.466467E-05	0.0000	H	9.861358E-06	2.463295E-05	0.0000
CH_2O	1.777633E-07	4.451404E-07	0.0000	CH_2O	2.719067E-07	6.792030E-07	0.0000
CHNO	1.649310E-08	4.130070E-08	0.0000	CHNO	2.889936E-08	7.218849E-08	0.0000
CNO	8.222593E-09	2.059035E-08	0.0000	CNO	2.007627E-08	5.014905E-08	0.0000
N	3.488577E-09	8.735813E-09	0.0000	N	9.259689E-09	2.313002E-08	0.0000
C(gr)	1.990688E-10	4.984920E-10	0.0000	N_2O	3.636584E-10	9.083920E-10	0.0000
N_2O	1.561364E-10	3.909841E-10	0.0000	C(gr)	2.091857E-10	5.225305E-10	0.0000

NO_2	2.346217E-11	5.875206E-11	0.0000	NO_2	6.503371E-11	1.624494E-10	0.0000

5a				**5b**			
Detonation Products	mol/mol	mol/kg	Mol %	Detonation Products	mol/mol	mol/kg	Mol %
C(d)	9.438500E00	1.845469E01	35.6171	N_2	9.674752E00	1.888007E01	37.0438
N_2	9.218725E00	1.802497E01	34.7877	C(d)	8.798533E00	1.717015E01	33.6889
H_2O	3.784262E00	7.399202E00	14.2803	H_2O	3.792490E00	7.400962E00	14.5211
NH_3	2.557664E00	5.000889E00	9.6516	NH_3	2.645062E00	5.161781E00	10.1277
CH_4	7.713203E-01	1.508129E00	2.9107	CH_4	5.880342E-01	1.147536E00	2.2515
C_2H_6	3.215654E-01	6.287426E-01	1.2135	H_2	2.501983E-01	4.882566E-01	0.9580
H_2	2.702594E-01	5.284264E-01	1.019	C_2H_6	2.350094E-01	4.644701E-01	0.9113
CH_2O_2	7.819018E-02	1.528818E-01	0.2951	CH_2O_2	7.922424E-02	1.546044E-01	0.3033
CO	3.056332E-02	5.975911E-02	0.1153	CO	2.632931E-02	5.138108E-02	0.1008
CO_2	1.424277E-02	2.784826E-02	0.0537	CO_2	1.124582E-02	2.194597E-02	0.0431
C_2H_4	9.940859E-03	1.943692E-02	0.0375	C_2H_4	8.222366E-03	1.604577E-02	0.0315
HCN	3.862434E-03	7.552048E-03	0.0146	HCN	3.928827E-03	7.667020E-03	0.0150
N_2H_4	5.043249E-04	9.860842E-04	0.0019	N_2H_4	7.435408E-04	1.451004E-03	0.0028
CH_3OH	3.079444E-04	6.021102E-04	0.0012	CH_3OH	2.406324E-04	4.695890E-04	0.0009
NH_2	1.479471E-05	2.892745E-05	0.0001	NH_2	1.896272E-05	3.641989E-05	0.0001
H	3.953223E-06	7.729564E-06	0.0000	H	4.906934E-06	9.575777E-06	0.0000
CH_2O	3.000284E-07	5.866323E-07	0.0000	CH_2O	1.939807E-07	3.785494E-07	0.0000
CHNO	3.212872E-08	6.281987E-08	0.0000	CHNO	2.032405E-08	3.944195E-08	0.0000
CNO	4.291003E-09	8.390010E-09	0.0000	CNO	5.981160E-09	1.167210E-08	0.0000
N	9.306557E-10	1.819670E-09	0.0000	N	2.932220E-09	4.084873E-09	0.0000
C(gr)	2.506000E-10	4.899872E-10	0.0000	C(gr)	2.082187E-10	4.063342E-10	0.0000
N_2O	1.021229E-10	1.996764E-10	0.0000	N_2O	1.338515E-10	2.612084E-10	0.0000
NO_2	5.711419E-12	1.116729E-11	0.0000	NO_2	1.147823E-11	2.239952E-11	0.0000

5. References.

1. Dippold, A. A.; Klapotke, T. M. Synthesis and Characterization of Bis(triaminoguanidinium) 5,5'-Dinitrimino-3,3'-azo-1H-1,2,4-triazolate – A Novel Insensitive Energetic Material. Z. Anorg. Allg. Chem. 2011, 637, 1181–1193

2. X Chen, Z Q Cuo, C Zhang. Constructing a 3D-layered energetic metal– organic framework with the strong stacking interactions of hydrogen-bridged rings: the way to an insensitive high energy complex. CrystEngComm, 2020, 22, 5436–5446