Electronic Supplementary Material (ESI) for CrystEngComm.

N-methylene-C bridged tetrazole and 1,2,4-triazole energetic salts as promising primary explosives

Lingfeng Zhang, [a] *Yu Wang,* [b] *Yefeng Wang*, [a] *Shuai Liu*, [a] *Na Zhang*, [b] *Mingmin Yang*, [c] *Haixia Ma,* [a] *Zhaoqi Guo**,[a]

[a] School of Chemical Engineering / Xi'an Key Laboratory of Special Energy Materials, Northwest University, Xi'an 710069, Shaanxi, P. R. China.

[b] Xi'an North Hui An Chemical Industries Co. Ltd, Xi'an 710302，P. R. China.

[c] State Key Laboratory of NBC Protection for Civilian, Beijing, 102205, P. R. China

Table of Contents

1. General methods

All the reagents were obtained from commercial sources and used without further purification. TGA measurements were carried out on a METTLER TOLEDO TGA/DSC 3+ instrument with a heating rate of 10 K·min^{-1} under an argon atmosphere at a flow rate of 50 ml·min^{-1}. DSC were determined on a METTLER TOLEDO DSC 3 at a heating rate of 10 °C·min^{-1} in a N_2 atmosphere with a flow rate of 50 mL·min^{-1} under ambient atmospheric pressure. Impact sensitivities (IS) were measured on a home-made device according to the UN Recommendations on the Transport of Dangerous Goods, Manual of Tests and Criteria. Single-crystal X-ray diffraction patterns of complexes **2**, **3**, **4**, **6** and **7** were recorded on a Bruker APEX-II diffractometer with highly oriented graphite crystal monochromated Mo Kα radiation (λ = 0.71073 Å). The structures were solved by direct methods and refined by full-matrix least squares techniques based on F^2. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were added according to the theoretical models and refined isotropically. The CCDC numbers of **2**, **3**, **4**, **6** and **7** are 2084803, 2084791, 2084806, 2084805 and 2084804.

2. Synthesis of compound 1

BrCN (6.87 g64.84 mmol) was dissolved in 100 mL anhydrous acetonitrile. To this solution was added NaN_3 (21.07g0.32mol) portion wise at 0°C. After stirring at 0–5 °C for 4h, the reaction mixture was filtered. Ainoacetonitrile hydrochloride (2.00 g, 21.62 mmol) was dissolved in 10 mL water and NaOH (0.86 g，21.62 mmol) was added at 0°C. This solution was added to the filtrate dropwise at 0°C. It was allowed to react for 36h and the temperature was slowly raised to room temperature. The product was recrystallized form acetonitrile. Yield 68%, m.p. 170~172 °C.

^{1}H NMR (500 MHz, [D_6]DMSO): δ= 5.48, 7.09 ppm; ^{13}C NMR (125 MHz, [D_6] DMSO): δ= 33.3, 114.6, 155.5 ppm; IR (KBr): $\tilde{\nu}$ = 3465, 2785, 1605, 1518, 1472, 1416, 1349, 1246, 1118, 1025, 812, 736, 657 cm^{-1}; elemental analysis (%) $C_3H_4N_6$ (124.11 g·mol^{-1}): C 29.01, H 3.22, N 67.67; found: C 29.00, H 3.24, N 67.66.

3. Hydrogen bonds present for 2, 3, 4, 6 and 7

Table S1. Hydrogen bonds present in **2**

D–H···A	d(D–H)/Å	d(H–A)/Å	d(D–A)/Å	D–H–A/°
N5–H5B···O1	0.871	2.094	2.950	167.058
O2–H2···N1	0.985	1.653	2.621	166.591

Table S2. Hydrogen bonds present in **3**

D–H···A	d(D–H)/Å	d(H–A)/Å	d(D–A)/Å	D–H–A/°
N8–H8A···N1	0.910	2.267	2.993	136.511
N10–H10B···N6	0.874	2.115	2.972	166.290
N10–H10A···N2	0.862	2.243	3.083	164.674
N8–H8A···N5	0.860	2.277	3.003	142.247

Table S3. Hydrogen bonds present in **4**

D–H···A	d(D–H)/Å	d(H–A)/Å	d(D–A)/Å	D–H–A/°
N10–H10A···O6	0.880	1.999	2.862	166.360

N6−H6···O4	0.880	2.037	2.844	151.880
N1−H1···O1	0.880	1.789	2.642	162.853
N10−H10B···O3	0.880	2.116	2.964	161.834
N9−H9B···O5	0.881	2.288	3.149	165.592
N8−H8A···O3	0.880	2.345	3.122	147.451
N6−H6···O2	0.880	2.398	2.877	114.513
N8−H8B···O1	0.880	2.092	2.910	154.129

Table S4. Hydrogen bonds present in **6**

D−H···A	d(D−H)/Å	d(H−A)/Å	d(D−A)/Å	D−H−A/°
N1−H1···O1	0.880	2.285	2.962	108.138
N1−H1···O6	0.880	2.096	2.960	167.114
N12−H12C···N10	1.074	1.861	2.841	149.809
N12−H12A···O5	0.881	2.237	3.104	168.094
N12−H12B···O2	0.880	1.914	2.778	167.262
O6−H6A···O7	0.868	1.958	2.826	178.537
O7−H7B···N5	0.871	2.121	2.931	154.538
O7−H7A···O3	0.870	2.164	2.956	151.176
O5−H5···N7	0.840	1.823	2.654	169.403

Table S5. Hydrogen bonds present in **7**

D−H···A	d(D−H)/Å	d(H−A)/Å	d(D−A)/Å	D−H−A/°
O5−H5A···N5	0.865	2.083	2.945	174.262
O5−H5B···O2	0.835	2.255	3.048	158.802
O6−H6B···O4	0.806	2.897	3.270	110.749
O6−H6A···N10	0.804	2.236	2.997	158.226

4. Bond lengths (Å) and angles (°) for 2, 3, 4, 6 and 7

Table S6. Selected bond lengths (Å) and angles (°) for **2**

Compound 2			
O2C3	1.3067(18)	C1N4C2	130.50(13)
O1C3	1.2154(19)	N3N2N1	110.92(12)
N3N4	1.3656(18)	N2N3N4	106.31(12)
N4C1	1.3456(19)	C1N1N2	106.51(13)
N4C2	1.4485(19)	O2C3C2	111.36(13)
N2N3	1.2861(19)	O1C3O2	125.56(14)
N2N1	1.3650(18)	O1C3C2	123.08(13)
N1C1	1.328(2)	N4C1N5	125.55(14)
N5C1	1.346(2)	N1C1N4	107.60(13)
C3C2	1.511(2)	N1C1N5	126.85(15)
N3N4C2	120.40(12)	N4C2C3	111.30(12)
C1N4N3	108.66(12)		

Table S7. Selected bond lengths (Å) and angles (°) for **3**

Compound 3			
N7N9	1.3960(17)	N5C3	1.2984(18)
N7C3	1.3669(17)	N8H8A	0.8600
N7C4	1.3695(18)	N8H8B	0.8600
N4N3	1.3604(18)	N8C4	1.337(2)
N4C1	1.3458(19)	N9H9A	0.91(3)
N4C2	1.4469(18)	N9H9B	0.93(3)
N10H10A	0.8616	N6C4	1.3151(18)
N10C4	1.3548(19)	N1N2	1.359(2)
N10H10B	0.87(3)	N1C1	1.3295(19)
N3N2	1.282(2)	C3C2	1.490(2)
N5N6	1.4047(19)	C2H2A	0.9700
C3N7N9	124.58(12)	C2H2B	0.9700
C3N7C4	105.70(11)	H10AN10H10B	122.2
N3N4C2	120.64(13)	C4N10H10A	109.6
C1N4N3	108.40(12)	C4N10H10B	111.3(17)
C1N4C2	130.96(13)	N2N3N4	105.95(13)
H8AN8H8B	120	C3N6N6	107.42(12)
C1N8H8A	120	C4N6N5	107.14(12)
C1N8H8B	120	C1N1N2	105.37(13)
N7N9H9A	108.1(16)	N3N2N1	112.08(13)
N7N9H9B	107.9(19)	N7C3C2	123.10(12)
H9AN9H9B	109.(2)	N5C3N7	110.23(12)
N0C4N7	123.92(13)	N5C3C2	126.66(13)
N6C4N7	109.50(12)	N1C1N8	126.05(14)
N6C4N10	126.52(13)	N4C2C3	111.17(11)
N8C1N4	125.69(14)	N4C2H2A	109.4
N7C1N4	108.20(14)	N4C2H2B	109.4
C3C2H2B	109.4	C3C2H2A	109.4
H2AC2H2B	108		

Table S8. Selected bond lengths (Å) and angles (°) for **4**

Compound 4			
O1N11	1.2669(19)	N7C3	1.375(2)
O4N12	1.2676(19)	N7C4	1.357(2)
O6N12	1.2583(19)	N1N2	1.357(2)
O2N11	1.2339(19)	N1C1	1.337(2)
O3N11	1.2537(18)	N6N5	1.386(2)
O5N12	1.2350(19)	N6C4	1.329(2)
N4N3	1.3714(19)	N8C1	1.312(2)
N4C1	1.343(2)	N10C4	1.316(2)
N4C2	1.468(2)	N5C3	1.296(2)
N7N9	1.3982(18)	N3N2	1.272(2)

C3C2	1.490(2)	C1N4N3	109.69(13)
N3N4C2	119.88(13)	C1N4C2	130.43(13)
C3N7N9	124.30(13)	C4N7N9	128.49(14)
C4N7C3	107.19(13)	C1N1N2	109.93(14)
O6N12O4	119.13(14)	O5N12O4	120.89(14)
O5N12O6	119.98(14)	C4N6N5	112.34(13)
O2N11O1	119.68(14)	O2N11O3	121.29(14)
O3N11O1	119.03(14)	C3N5N6	103.75(13)
N2N3N4	107.42(13)	N3N2N1	108.62(13)
N1C1N4	104.32(14)	N8C1N4	128.68(15)
N8C1N1	126.99(15)	N7C3C2	122.81(14)
N5C3N7	111.60(14)	N5C3C2	125.47(15)
N6C4N7	105.11(14)	N10C4N7	126.84(15)
N10C4N6	128.04(15)	N4C2C3	110.62(13)

Table S9. Selected bond lengths (Å) and angles (°) for **6**

Compound 6			
O3N11	1.250(7)	O5N12	1.419(7)
O5H5	0.8400	O2N9	1.266(7)
O4N11	1.240(7)	N7C4	1.343(8)
O7H7A	0.8701	N7C3	1.337(8)
O7H7B	0.8705	N10N11	1.329(7)
N4N3	1.350(7)	N10C4	1.355(8)
N4C1	1.342(8)	N12H12A	0.8806
N4C2	1.457(8)	N12H12B	0.8798
N5N6	1.384(8)	N12H12C	1.08(10)
N5C3	1.306(8)	O6H6A	0.8689
O1N9	1.241(8)	O6H6B	0.8701
N1H1	0.8800	C3C2	1.496(9)
N1N2	1.365(8)	C2H2A	0.9900
N1C1	1.327(8)	C2H2B	0.9900
N6C4	1.369(8)	N8N9	1.297(8)
N3N2	1.283(8)	N8C1	1.368(8)
N12O5H5	109.5	C1N1N2	106.4(5)
H7AO7H7B	109.5	C4N6N5	108.2(5)
N3N4C2	119.8(5)	N2N3N4	105.8(5)
C1N4N3	109.9(5)	N9N8C1	117.0(6)
C1N4C2	130.3(5)	C3N7C4	104.1(5)
C3N5N6	103.3(5)	N3N2N1	111.1(5)
N2N1H1	126.8	N11N10C4	117.6(6)
C1N1H1	126.8	O3N11N10	122.1(6)
O4N11O3	122.0(6)	O5N12H12A	109
O4N11N10	115.8(5)	O5N12H12B	110.6
O2N9N8	115.8(6)	O5N12H12C	115.(6)

O1N9O2	119.5(6)	H12AN12H12B	109.5
O1N9N8	124.7(6)	H12AN12H12C	101.5
H12BN12H12C	111.1	N7C4N10	119.4(6)
H6AO6H6B	104.6	N10C4N6	131.8(6)
N7C4N6	108.8(6)	N5C3N7	115.5(6)
N5C3C2	121.4(6)	N4C2C3	113.7(5)
N7C3C2	123.0(6)	N4C2H2A	108.8
N4C1N8	116.9(6)	N4C2H2B	108.8
N1C1N4	106.8(6)	C3C2H2A	108.8
N1C1N8	136.4(6)	C3C2H2B	108.8
H2AC2H2B	107.7		

Table S10. Selected bond lengths (Å) and angles (°) for **7**

Compound 7			
K2K2i	4.0899(18)	K2O6i	2.7678(18)
K2K2ii	4.0899(18)	K2O6	2.6787(17)
K2K2iii	4.645(3)	K2O4iii	2.8596(19)
K2O4iv	2.8358(17)	K2O4	2.7334(19)
K2O3iii	2.9326(18)	K2N7v	3.0597(19)
K2N11iii	3.289(2)	K1N1	2.8307(19)
K2N3v	3.013(2)	K1N9vi	3.258(2)
K2H6B	3.08(3)	O3N11	1.2563(18)
K1K1i	4.0899(18)	O6H6A	0.80(3)
K1K1ii	4.0899(18)	O6H6B	0.81(3)
K1K1vi	4.779(2)	O4N11	1.255(2)
K1O5i	2.7965(19)	O5H5A	0.86(3)
K1O5	2.7313(18)	O5H5B	0.83(4)
K1O2vi	2.8640(19)	O2N9	1.259(2)
K1O2vii	2.827(2)	N4N3	1.3390(19)
K1O1vi	2.8819(19)	N4C1	1.348(2)
K1O1	2.775(2)	N4C2	1.457(2)
N5N6	1.359(2)	N5C3	1.312(2)
N7C4	1.338(2)	N7C3	1.357(2)
N6C4	1.343(2)	N11N10	1.312(2)
N10C4	1.381(2)	O1N9	1.235(2)
N1N2	1.358(2)	N1C1	1.333(2)
N8N9	1.313(2)	N8C1	1.364(2)
N2N3	1.293(2)	C3C2	1.486(2)
C2H2A	0.9900	C2H2B	0.9900
K2iiK2K2iii	79.19(3)	O4ivK2O4iii	75.27(5)
K2iK2K2iii	100.81(3)	O4ivK2N7v	116.61(5)
K2iK2K2ii	180	O3iiiK2N7v	112.77(5)
K2iiK2H6B	49.0(5)	O4ivK2N11iii	79.13(5)
K2iK2H6B	131.0(5)	O3iiiK2N11iii	22.37(4)

K2iiiK2H6B	76.2(5)	O4ivK2N3v	71.29(5)
O4ivK2K2ii	134.19(3)	O3iiiK2N3v	66.34(5)
O3iiiK2K2iii	72.78(4)	O4ivK2H6B	163.1(5)
O4ivK2K2iii	87.96(4)	O3iiiK2H6B	90.6(5)
O4ivK2K2i	45.81(4)	O6K2K2i	137.84(4)
O3iiiK2K2ii	43.90(3)	O6K2K2iii	87.42(5)
O3iiiK2K2i	136.10(3)	O6iK2K2iii	103.51(5)
O4ivK2O3iii	90.29(5)	O6K2K2ii	42.16(4)
O6iK2K2ii	139.49(3)	O6iK2K2i	40.51(3)
O6K2O3iii	85.94(5)	O6K2O4iv	174.74(4)
O6iK2O4iv	86.20(5)	O6iK2O3iii	175.01(4)
O6K2O6i	97.33(6)	O6iK2O4iii	131.31(5)
O6K2O4	75.61(5)	O6K2O4iii	99.47(6)
O6iK2N7v	72.04(5)	O6K2N7v	68.35(5)
O6iK2N11iii	152.77(4)	O6K2N11iii	96.09(5)
O6K2N3v	110.35(5)	O6iK2N3v	115.65(5)
O6K2H6B	14.0(5)	O6iK2H6B	91.7(5)
O4iiiK2K2i	109.81(4)	O4iiiK2K2ii	70.19(4)
O4K2K2i	87.95(5)	O4K2K2ii	92.05(5)
O4K2K2iii	34.72(3)	O4K2K2	32.99(3)
O4K2O3iii	104.39(5)	O4iiiK2O3iii	44.07(4)
O4K2O4iv	101.85(5)	O4K2O6i	72.94(5)
O4K2O4iii	67.71(5)	O4iiiK2N7v	156.07(4)
O4K2N7v	124.92(4)	O4K2N11iii	87.69(5)
O4iiiK2N11iii	22.18(4)	O4iiiK2N3v	100.49(5)
O4K2N3v	167.85(4)	O4iiiK2H6B	93.9(5)
O4K2H6B	61.7(5)	N7vK2K2iii	154.09(3)
N7vK2K2i	91.89(4)	N7vK2K2ii	88.11(4)
N7vK2N11iii	135.13(5)	N7vK2H6B	78.4(5)
N11iiiK2K2ii	57.84(4)	N11iiiK2K2i	122.16(4)
N11iiiK2K2iii	53.58(4)	N11iiiK2H6B	95.8(5)
N3vK2K2i	93.74(5)	N3vK2K2ii	86.26(5)
N3vK2K2iii	133.42(4)	N3vK2N7v	67.09(5)
N3vK2N11iii	81.22(5)	N3vK2H6B	124.2(5)
K1iiK1K1i	180	K1iK1K1vi	91.53(3)
K1iiK1K1vi	88.47(3)	O5iK1K1vi	133.17(4)
O05K1K1vi	131.34(4)	O5iK1K1i	41.67(4)
O5iK1K1ii	138.33(4)	O5K1K1i	137.10(4)
O5K1K1ii	42.90(4)	O5K1O5i	95.43(6)
O5iK1O2vi	135.05(5)	O5K1O2vii	134.20(5)
O5K1O6vi	69.02(5)	O5iK1O2vii	68.67(5)
O5iK1O1vi	146.67(5)	O5K1O1	143.69(5)
O5K1O1vi	108.62(6)	O5K1N1	105.36(6)
O5iK1N1	75.32(6)	O5K1N9vi	90.46(5)

O5iK1N9vi	143.26(5)	O2viK1K1ii	135.58(4)
O2viK1K1vi	75.51(4)	O2viiK1K1vi	77.58(4)
O2viK1K1ii	43.70(4)	O2viK1K1i	136.30(4)
O2viiK1K1i	44.42(4)	O2viiK1O2vi	91.88(5)
O2viiK1O1vi	78.00(6)	O2viK1O1vi	44.24(5)
O2viiK1N1	110.92(5)	O2viiK1N9vi	81.34(6)
O2viK1N9vi	22.57(4)	O1K1K1i	70.98(5)
O1K1K1ii	109.02(5)	O1viK1K1vi	31.68(3)
O1viK1K1i	110.98(5)	O1viK1K1ii	69.02(5)
O1K1K1vi	33.05(3)	O1K1O5i	108.08(5)
O1K1O2vii	81.12(5)	O1K1O2vi	108.24(5)
O1K1O1vi	64.73(5)	O1K1N1	57.12(5)
O1viK1N9vi	22.14(4)	O1K1N9vi	86.86(5)
N1K1K1ii	110.49(5)	N1K1K1vi	88.09(5)
N1K1K1i	69.51(5)	N1K1O2vi	148.48(5)
N1K1O1vi	117.87(5)	N1K1N9vi	137.51(5)
N9viK1K1vi	53.81(4)	N9viK1K1ii	57.15(4)
N9viK1K1i	122.85(4)	K2ivO3K2iii	90.29(5)
N11O3K2iv	120.39(9)	N11O3K2iii	94.98(9)
K2O6K2ii	97.33(5)	K2O6H6A	112.(2)
K2O6H6A	115.(2)	K2O6H6B	112.6(19)
K2O6H6B	108.1(19)	H6AO6H6B	110.(3)
K2O4K2iii	112.29(5)	N11O4K2	139.34(10)
N11O4K2iii	98.52(9)	K1O5K1ii	95.43(6)
K1iiO5H5A	110.0(18)	K1O5H5A	124.5(18)
K1iiO5H5B	101.(2)	K1O5H5B	117.(2)
H5AO5H5B	106.(3)	K1viiO2K1vi	91.88(5)
N9O2K1vi	96.58(10)	N9O2K1vii	117.68(12)
N3N4C1	109.16(13)	N3N4C2	121.38(13)
C1N4C2	129.40(14)	C3N5N6	102.65(14)
C4N7K2v	137.27(11)	C4N7C3	102.44(13)
C3N7K2v	120.29(10)	C4N7N8	109.80(13)
O3N11K2iii	62.66(8)	O311N10	123.46(14)
O4N11K2iii	59.30(8)	O4N11O3	119.89(13)
O4N11N10	116.65(13)	N10N11K2iii	164.61(10)
N11N10C4	116.68(13)	K1O1K1vi	115.27(5)
N9O1K1vi	96.31(11)	N9O1K1	148.35(12)
N2N1K1	121.11(10)	C1N1K1	131.26(11)
C1N11N2	105.18(13)	N9N8C1	116.73(14)
N3N2N1	111.84(13)	N4N3K2v	121.76(10)
N2N3K2v	126.72(11)	N2N3N4	105.97(13)
O2N9K1vi	60.84(9)	O2N9N8	115.19(14)
O1N9K1vi	61.55(9)	O1N9O2	120.31(15)
O1N9N8	124.50(15)	N8N9K1vi	164.07(12)

N7C4N6	109.76(14)	N7C4N10	119.50(14)
N6C4N10	130.73(14)	N5C3N7	115.35(15)
N5C3C2	121.19(15)	N7C3C2	123.46(14)
N4C1N8	115.84(14)	N1C1N4	107.84(14)
N1C1N8	136.28(15)	N4C2C3	111.47(13)
N4C2H2A	109.3	N4C2H2B	109.3
C3C2H2A	109.3	C3C2H2B	109.3
H2AC2H2B	108		

(i) -1+x, y, z; (ii) 1+x, y, z; (iii) 2-x, 2-y, 1-z; (iv) 1-x, 2-y, 1-z; (v) 1-x, 1-y, 1-z; (vi) 1-x, -y, -z; (vii) -x, -y, -z

5. Detailed calculation procedure of IGM analyses and the iso-surfaces of IGM analyses of 2(a), 3(b), 4(c), 6(d) and 7(e)

Single point calculations of each crystal repeat units were performed at the B3LYP-D3(BJ)/TZVP level of theory using the ORCA quantum-chemistry program package [1]. The wave function files generated from the single-point calculations were loaded with Multiwfn and the lattice point data for the δg_inter function was generated [2]. Finally, the IGM isosurface maps were generated using VMD software.

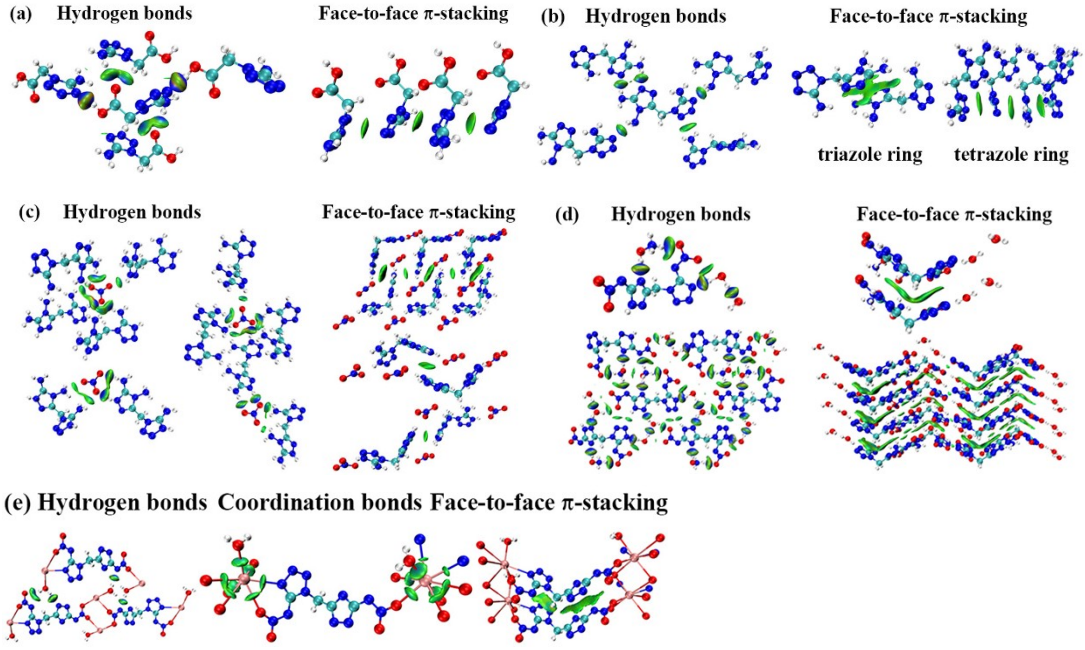

Figure. S1 The iso-surfaces of IGM analyses of **2**(a), **3**(b), **4**(c), **6**(d) and **7**(e) adopted from their unit cells.

6. Detailed calculation of enthalpies of formation

Table S11. Detailed calculation of enthalpies of formation of complexes **4**, **6** and **7**

	Calc. Density (g/cm^3)	**Formula**	**Q_v (kJ / mol)**
4	1.715	$C_4H_{10}N_{12}O_6$	3999
6	1.724	$C_4H_{11}N_{12}O_7$	4003
7	1.838	$C_4H_6K_2N_{11}O_6$	2301
	Δn_g	**$\Delta_c H$ (kJ/mol)**	**$\Delta_f H$ (kJ/mol)**

$C_4H_{10}N_{12}O_6 + 3.5\ O_2 = 5H_2O + 4\ CO_2 + 6\ N_2$	6.5	4027.1	667.7
$C_4H_{11}N_{12}O_7 + 3.25\ O_2 = 5.5\ H_2O + 4\ CO_2 + 6\ N_2$	6.75	4030.7	473.5
$C_4H_6K_2N_{11}O_6 + 3\ O_2 = 3H_2O + 4\ CO_2 + 5.5\ N_2 + 1\ K_2O$	6.5	2324.1	272.5

The standard enthalpies of formation (Δ_fH^θ) were calculated according to Hess's law:

Δ_fH ($C_4H_{10}N_{12}O_6$, s) = 5 Δ_fH (H_2O, l) + Δ_fH (CO, g) + 3 Δ_fH(C, s)+6 Δ_fH(N_2, g)-Δ_cH ($C_4H_{10}N_{12}O_6$)

Δ_fH ($C_4H_{11}N_{12}O_7$, s) = 5.5 Δ_fH (H_2O, l) + 1.5 Δ_fH (CO, g) + 2.5 Δ_fH (C, s) + 6 Δ_fH (N_2, g) - Δ_cH ($C_4H_{11}N_{12}O_7$)

Δ_fH ($C_4H_6K_2N_{11}O_6$, s) = 3Δ_fH (H_2O, l) + Δ_fH(K_2O, g) + 2 Δ_fH (CO, g) + 2 Δ_fH (C, s) + 5.5 Δ_fH (N_2, g) - Δ_cH ($C_4H_6K_2N_{11}O_6$)

7. Schematic diagram of electric initiation device

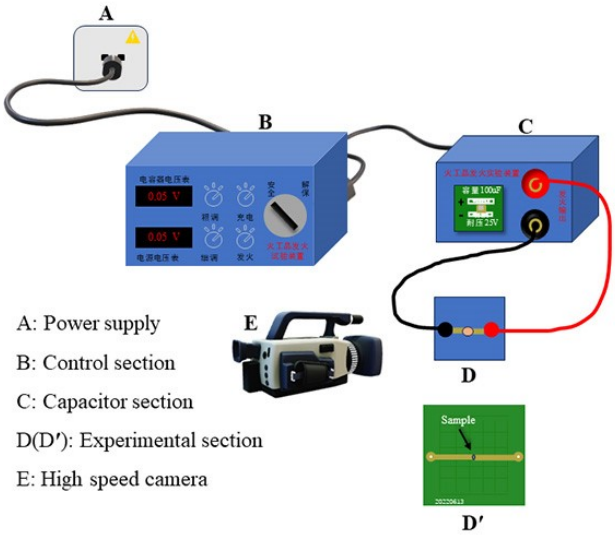

Figure S2 The schematic diagram of the device and some of its parameters

8. Gif picture of ignition of RDX

Figure S3 The picture of ignition of RDX

9. References.

[1] Neese F. Software update: The ORCA program system—Version 5.0[J]. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12(5): e1606.

[2] Lu T, Chen Q. Independent gradient model based on Hirshfeld partition: A new method for visual study of interactions in chemical systems. *J. Comput. Chem.*, **2022**, 43(8): 539-555. DOI: 10.1002/jcc.2681212