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Strong Intermolecular Interactions Induced Methylene-Bridged Asymmetric Heterocyclic Explosives

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Table S1−3. Hydrogen bonds present for **4, 5** and **6**

Table S1. Hydrogen bonds present in **4**

D−H···A	d(D−H)/Å	d(H−A)/Å	d(D−A)/Å	D−H−A/°
N1-H1	0.847	2.559	3.019	115.27
N1-H1	0.847	2.096	2.561	114.08
N1-H1	0.847	2.629	3.451	163.75
N6-H6	0.879	2.031	2.857	156.27
C2-H2A	0.990	2.444	3.012	115.95
C2-H2A	0.990	2.546	3.387	142.81
C2-H2B	0.990	2.479	3.181	127.56
C2-H2B	0.990	2.393	3.083	126.22

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

Table S2. Hydrogen bonds present in **5**

D−H···A	d(D−H)/Å	d(H−A)/Å	d(D−A)/Å	D−H−A/°
C3-H3B	0.968	2.500	3.422	159.22
N11-H11A	0.933	1.944	2.872	173.15
N11-H11B	0.931	2.073	2.900	147.12
N11-H11B	0.931	2.664	3.232	119.98
N11-H11B	0.931	2.596	3.318	134.70
N11-H11C	0.934	2.158	3.091	176.88
N11-H11D	0.860	2.496	2.999	118.13
N11-H11D	0.860	2.436	3.175	144.42
N12-H12A	0.905	2.040	2.940	172.90
N12-H12A	0.905	2.634	3.211	122.38
N12-H12A	0.905	2.678	3.481	148.43
N12-H12B	0.924	1.971	2.827	153.25
N12-H12C	0.842	2.300	2.855	123.83
N12-H12C	0.842	2.217	2.956	146.59
N12-H12D	0.924	2.626	3.205	121.27
N12-H12D	0.924	2.115	2.972	153.75

Table S3. Hydrogen bonds present in **6**

D−H···A	d(D−H)/Å	d(H−A)/Å	d(D−A)/Å	D−H−A/°
C2-H2A	0.990	2.551	3.506	162.04
C2-H2B	0.990	2.699	3.675	168.56

Table S4−6. Selected bond lengths (Å) and angles (°) for **4, 5** and **6**

Table S4. Selected bond lengths (Å) and angles (°) for **4**

Compound 4			
O3N10	1.234(3)	N4N3	1.364(3)

O2N10	1.233(3)	N4C1	1.351(4)
O4N8	1.233(3)	N4C2	1.451(4)
O5N8	1.244(3)	N3N2	1.276(3)
O1N5	1.432(3)	N2N1	1.365(3)
O1C4	1.337(3)	N1C1	1.349(4)
N8N7	1.362(3)	N6C3	1.372(4)
N7C1	1.334(4)	N6C4	1.335(3)
N9N10	1.360(3)	N5C3	1.285(3)
N9C4	1.317(4)	C3C2	1.486(4)
C4O1N5	108.2(2)	C1N1N2	110.6(2)
O4N8O5	123.2(2)	C4N6C3	106.1(2)
O4N8N7	114.8(2)	C3N5O1	104.1(2)
O5N8N7	121.9(2)	N6C3C2	122.7(2)
C1N7N8	114.0(2)	N5C3N6	112.8(2)
C4N9N10	116.1(2)	N5C3C2	124.5(3)
O3N10N9	122.3(2)	N9C4O1	115.0(2)
O2N10O3	123.6(2)	N9C4N6	136.4(3)
O2N10N9	114.1(2)	N6C4O1	108.7(2)
N3N4C2	121.0(2)	N7C1N4	120.4(3)
C1N4N3	110.9(2)	N7C1N1	136.7(3)
C1N4C2	127.8(2)	N1C1N4	102.9(2)
N2N3N4	107.6(2)	N4C2C3	110.8(2)
N3N2N1	108.0(2)		

Table S5. Selected bond lengths (Å) and angles (°) for **5**

Compound 5			
O4N10	1.275(2)	N5C4	1.353(2)
O5N10	1.242(2)	N5C3	1.457(2)
O3N1	1.255(2)	N9C4	1.372(2)
O2N1	1.251(2)	N8C4	1.332(2)
O1N4	1.423(2)	C2C3	1.500(3)
O1C1	1.356(2)	C3H3A	0.99(2)
N10N9	1.322(2)	C3H3B	0.97(2)
N3C1	1.313(3)	N11H11A	0.93(3)
N3C2	1.378(2)	N11H11B	0.93(3)
N6N7	1.295(2)	N11H11C	0.93(3)
N6N5	1.352(2)	N11H11D	0.86(3)
N4C2	1.297(3)	N12H12A	0.91(3)
N7N8	1.364(2)	N12H12B	0.92(3)
N1N2	1.330(2)	N12H12C	0.84(3)
N2C1	1.354(3)	N12H12D	0.924(19)
C1O1N4	106.42(15)	N2C1O1	110.15(17)
O4N10N9	115.23(15)	N3C2C3	120.93(18)
O5N10O4	119.46(15)	N4C2N3	116.34(18)

O5N10N9	125.27(16)	N4C2C3	122.72(18)
C1N3C2	101.81(17)	N5C3C2	111.23(17)
N7N6N5	106.51(15)	N5C3H3A	110.5(12)
C2N4O1	102.59(15)	N5C3H3B	108.3(12)
N6N7N8	110.96(15)	C2C3H3A	108.6(12)
O3N1N2	123.31(16)	C2C3H3B	110.2(12)
O2N1O3	120.56(17)	H3AC3H3B	107.9(18)
O2N1N2	116.12(17)	H11AN11H11B	111.(2)
N1N2C1	117.54(17)	H11AN11H11C	108.(2)
N6N5C4	108.74(15)	H11AN11H11D	110.(2)
N6N5C3	121.22(16)	H11BN11H11C	107.(2)
C4N5C3	130.01(17)	H11BN11H11D	110.(2)
N10N9C4	115.08(15)	H11CN11H11D	111.(2)
C4N8N7	106.12(16)	H12AN12H12B	117.(3)
N5C4N9	118.19(17)	H12AN12H12C	113.(3)
N8C4N5	107.66(16)	H12AN12H12D	106.(3)
N8C4N9	134.14(18)	H12BN12H12C	111.(3)
N3C1O1	112.83(17)	H12BN12H12D	97.(3)
N3C1N2	136.95(19)	H12CN12H12D	112.(3)

Table S6. Selected bond lengths (Å) and angles (°) for **6**

Complex 6			
K1O4^{ii}	2.718(2)	K2C4^{viii}	3.405(3)
K1O4^{iii}	2.7564(19)	O4N8	1.271(3)
K1O5	2.5964(19)	O5N8	1.247(3)
K1O5^{iii}	2.8798(19)	O1N5	1.426(3)
K1O2^{iv}	2.7880(19)	O1C4	1.355(3)
K1N8^{iii}	3.181(2)	O3N10	1.253(3)
K1N8^{ii}	3.256(2)	O2N10	1.257(3)
K1N7^{ii}	3.249(2)	N8N7	1.308(3)
K1N1	2.791(2)	N7C1	1.368(3)
K1N3^{v}	3.120(2)	N4N3	1.355(3)
K1N2^{vi}	3.073(2)	N4C1	1.353(3)
K2O4^{vii}	2.7468(19)	N4C2	1.450(3)
K2O1^{viii}	2.968(2)	N1N2	1.366(3)
K2O3^{ix}	2.848(2)	N1C1	1.334(3)
K2O3	2.690(2)	N9N10	1.322(3)
K2O2^{ix}	2.922(2)	N9C4	1.363(3)
K2N7^{vii}	3.425(2)	N3N2	1.293(3)
K2N9^{viii}	2.972(2)	N6C4	1.315(3)
K2N3^{x}	3.135(2)	N6C3	1.368(3)
K2N6	2.833(2)	N5C3	1.297(3)
K2N10^{ix}	3.280(2)	C3C2	1.507(4)

K2N5^{x}	3.110(2)	C2H2A	0.9900
N9^{viii}K2N5^{x}	154.95(6)	C2H2B	0.9900
O4^{ii}K1O4^{iii}	81.63(6)	N9^{viii}K2N10^{ix}	103.80(6)
O4^{iii}K1O5^{iii}	45.25(5)	N9^{viii}K2C4^{viii}	23.45(6)
O4^{ii}K1O5^{iii}	103.31(5)	N3^{x}K2N7^{vii}	94.49(6)
O4^{ii}K1O2^{iv}	87.62(6)	N3^{x}K2N10^{ix}	98.23(6)
O4^{iii}K1O2^{iv}	168.88(6)	N3^{x}K2C4^{viii}	165.54(6)
O4^{iii}K1N8^{iii}	23.34(5)	N6K2O1^{viii}	102.15(6)
O4^{ii}K1N8^{iii}	88.08(6)	N6K2O3^{ix}	135.63(6)
O4^{ii}K1N8^{ii}	22.32(5)	N6K2O2^{ix}	175.75(6)
O4^{iii}K1N8^{ii}	85.92(6)	N6K2N7^{vii}	114.89(6)
O4^{iii}K1N7^{ii}	105.64(6)	N6K2N9^{viii}	76.92(6)
O4^{ii}K1N7^{ii}	41.67(5)	N6K2N3^{x}	94.41(6)
O4^{ii}K1N1	154.78(6)	N6K2N10^{ix}	156.66(6)
O4^{iii}K1N1	113.49(6)	N6K2N5^{x}	87.95(6)
O4^{ii}K1N3^{v}	60.67(5)	N6K2C4^{viii}	83.02(6)
O4^{iii}K1N3^{v}	79.77(6)	N10^{ix}K2N7^{vii}	83.67(5)
O4^{ii}K1N2^{vi}	77.88(6)	N10^{ix}K2C4^{viii}	89.26(6)
O4^{iii}K1N2^{vi}	58.75(6)	N5^{x}K2N7^{vii}	146.41(6)
N10O3K2	140.56(16)	N5^{x}K2N3^{x}	57.75(6)
O5K1O4^{ii}	133.49(6)	N5^{x}K2N10^{ix}	82.38(6)
O5K1O4^{iii}	117.30(6)	N5^{x}K2C4^{viii}	136.02(6)
O5K1O5^{iii}	120.31(3)	C4^{viii}K2N7^{vii}	73.95(6)
O5K1O2^{iv}	72.45(6)	K1^{vii}O4K1^{vi}	98.37(6)
O5K1N8^{ii}	112.23(6)	K1^{vii}O4K2^{ii}	89.04(6)
O5^{iii}K1N8^{ii}	119.66(5)	K2^{ii}O4K1^{vi}	146.77(7)
O5^{iii}K1N8^{iii}	23.06(5)	N8O4K1^{vii}	103.40(14)
O5K1N8^{iii}	126.75(6)	N8O4K1^{vi}	97.41(14)
O5K1N7^{ii}	91.94(6)	N8O4K2^{ii}	112.37(14)
O5^{iii}K1N7^{ii}	142.86(5)	K1O5K1^{vi}	125.65(7)
O5K1N1	59.12(6)	N8O5K1	135.22(15)
O5K1N3^{v}	156.90(6)	N8O5K1^{vi}	92.15(13)
O5^{iii}K1N3^{v}	59.44(6)	N5O1K2^{xi}	135.24(14)
O5^{iii}K1N2^{vi}	102.03(6)	C4O1K2^{xi}	96.75(14)
O5K1N2^{vi}	78.04(6)	C4O1N5	106.21(19)
O2^{iv}K1O5^{iii}	136.24(6)	K2O3K2^{ix}	100.47(6)
O2^{iv}K1N8^{iii}	154.24(6)	N10O3K2^{ix}	98.69(15)
O2^{iv}K1N8^{ii}	85.20(6)	K1^{iv}O2K2^{ix}	84.25(5)
O2^{iv}K1N7^{ii}	67.34(6)	N10O2K1^{iv}	145.40(16)
O2^{iv}K1N1	75.63(6)	N10O2K2^{ix}	95.01(15)
O2^{iv}K1N3^{v}	92.50(6)	K1^{vi}N8K1^{vii}	80.12(5)
O2^{iv}K1N2^{vi}	121.73(6)	K1^{vii}N8K2^{ii}	69.77(4)
O4N8K2^{ii}	47.64(11)	K1^{vi}N8K2^{ii}	105.58(6)
N8^{iii}K1N8^{ii}	99.88(5)	O4N8K1^{vi}	59.24(12)

N8^{iii}K1N7^{ii}	122.42(6)	O4N8K1^{vii}	54.29(12)
O5N8O4	119.1(2)	O4N8N7	115.4(2)
N7^{ii}K1N8^{ii}	23.20(5)	O5N8K1^{vii}	134.85(15)
N1K1O5^{iii}	77.68(6)	O5N8K1^{vi}	64.79(12)
N1K1N8^{ii}	160.57(6)	O5N8K2^{ii}	144.63(16)
N1K1N8^{iii}	98.80(6)	O5N8N7	125.5(2)
N1K1N7^{ii}	138.77(6)	N7N8K1^{vii}	78.11(13)
N1K1N3^{v}	100.77(6)	N7N8K1^{vi}	154.81(16)
N1K1N2^{vi}	126.97(7)	N7N8K2^{ii}	78.49(13)
N3N4C2	122.0(2)	K1^{vii}N7K2^{ii}	70.01(4)
N3^{v}K1N8^{ii}	82.97(6)	N8N7K1^{vii}	78.70(13)
N3^{v}K1N8^{iii}	63.45(6)	N8N7K2^{ii}	79.55(13)
N3^{v}K1N7^{ii}	98.38(6)	N8N7C1	116.2(2)
N2^{vi}K1N8^{iii}	82.00(6)	C1N7K1^{vii}	142.47(17)
N2^{vi}K1N8^{ii}	61.41(6)	C1N7K2^{ii}	143.47(17)
N2^{vi}K1N7^{ii}	64.70(6)	C1N4N3	108.9(2)
N2^{vi}K1N3^{v}	125.06(6)	C1N4C2	129.1(2)
O4^{vii}K2O1^{viii}	116.13(5)	N2N1K1	125.69(16)
O4^{vii}K2O3^{ix}	127.02(6)	C1N1K1	125.00(16)
O4^{vii}K2O2^{ix}	84.45(6)	C1N1N2	105.6(2)
O4^{vii}K2N7^{vii}	39.46(5)	N10N9K2^{xi}	138.69(17)
O4^{vii}K2N9^{viii}	83.97(6)	N10N9C4	117.0(2)
O4^{vii}K2N3^{x}	60.20(6)	C4N9K2^{xi}	96.37(15)
O4^{vii}K2N6	96.59(6)	K1^{x}N3K2^{v}	75.54(5)
O4^{vii}K2N10^{ix}	106.72(6)	N4N3K1^{x}	128.17(15)
O4^{vii}K2N5^{x}	117.95(6)	N4N3K2^{v}	126.63(15)
O4^{vii}K2C4^{viii}	105.84(6)	N2N3K1^{x}	111.09(15)
O1^{viii}K2N7^{vii}	77.77(5)	N2N3K2^{v}	105.91(15)
O1^{viii}K2N9^{viii}	44.01(6)	N2N3N4	106.0(2)
O1^{viii}K2N3^{x}	163.41(6)	N1N2K1^{iii}	114.64(15)
O1^{viii}K2N10^{ix}	66.59(5)	N3N2K1^{iii}	123.85(16)
O1^{viii}K2N5^{x}	123.16(6)	N3N2N1	111.7(2)
O1^{viii}K2C4^{viii}	23.28(6)	C4N6K2	128.33(17)
O3K2O4^{vii}	152.45(6)	C4N6C3	101.4(2)
O3^{ix}K2O1^{viii}	68.42(6)	C3N6K2	129.74(17)
O3K2O1^{viii}	62.74(6)	O3N10K2^{ix}	59.14(13)
O3K2O3^{ix}	79.53(6)	O3N10O2	120.1(2)
O3^{ix}K2O2^{ix}	44.25(5)	O3N10N9	124.1(2)
O3K2O2^{ix}	118.84(6)	O2N10K2^{ix}	62.54(13)
O3^{ix}K2N7^{vii}	105.47(5)	O2N10N9	115.8(2)
O3K2N7^{vii}	135.40(6)	N9N10K2^{ix}	168.47(17)
O3K2N9^{viii}	78.19(6)	O1N5K2^{v}	101.10(13)
O3^{ix}K2N9^{viii}	111.73(6)	C3N5K2^{v}	122.49(17)
O3^{ix}K2N3^{x}	100.23(6)	C3N5O1	102.11(19)

O3K2N3^{x}	128.85(6)	N4C1N7	117.5(2)
O3K2N6	59.11(6)	N1C1N7	134.7(2)
O3K2N10^{ix}	97.88(6)	N1C1N4	107.8(2)
O3^{ix}K2N10^{ix}	22.18(5)	O1C4K2^{xi}	59.97(12)
O3K2N5^{x}	76.91(6)	O1C4N9	109.9(2)
O3^{ix}K2N5^{x}	66.16(6)	N9C4K2^{xi}	60.18(13)
O3^{ix}K2C4^{viii}	91.38(6)	N6C4K2^{xi}	145.59(18)
O3K2C4^{viii}	61.54(6)	N6C4O1	113.1(2)
O2^{ix}K2O1^{viii}	73.74(6)	N6C4N9	136.9(2)
O2^{ix}K2N7^{vii}	63.53(5)	N6C3C2	120.1(2)
O2^{ix}K2N9^{viii}	99.12(6)	N5C3N6	117.2(2)
O2^{ix}K2N3^{x}	89.69(6)	N5C3C2	122.7(2)
O2^{ix}K2N10^{ix}	22.44(5)	N4C2C3	111.7(2)
O2^{ix}K2N5^{x}	95.22(6)	N4C2H2A	109.300
O2^{ix}K2C4^{viii}	92.72(6)	N4C2H2B	109.300
N9^{viii}K2N7^{vii}	58.51(6)	C3C2H2A	109.300
N3^{v}K1N8^{iii}	63.45(6)	C3C2H2B	109.300
N3^{v}K1N7^{ii}	98.38(6)	H2AC2H2B	107.900
N2^{vi}K1N8^{iii}	82.00(6)	C1N7K1^{vii}	142.47(17)
N2^{vi}K1N8^{ii}	61.41(6)	C1N7K2^{ii}	143.47(17)
N2^{vi}K1N7^{ii}	64.70(6)	N3N4C2	122.0(2)
N2^{vi}K1N3^{v}	125.06(6)	C1N4N3	108.9(2)
O4^{vii}K2O1^{viii}	116.13(5)	C1N4C2	129.1(2)
O4^{vii}K2O3^{ix}	127.02(6)	N2N1K1	125.69(16)
O4^{vii}K2O2^{ix}	84.45(6)	C1N1K1	125.00(16)
O4^{vii}K2N7^{vii}	39.46(5)	C1N1N2	105.6(2)
O4^{vii}K2N9^{viii}	83.97(6)	N10N9K2^{xi}	138.69(17)
O4^{vii}K2N3^{x}	60.20(6)	N10N9C4	117.0(2)
O4^{vii}K2N6	96.59(6)	C4N9K2^{xi}	96.37(15)
O4^{vii}K2N10^{ix}	106.72(6)	K1^{x}N3K2^{v}	75.54(5)
O4^{vii}K2N5^{x}	117.95(6)	N4N3K1^{x}	128.17(15)
O4^{vii}K2C4^{viii}	105.84(6)	N4N3K2^{v}	126.63(15)
O1^{viii}K2N7^{vii}	77.77(5)	N2N3K1^{x}	111.09(15)
O1^{viii}K2N9^{viii}	44.01(6)	N2N3K2^{v}	105.91(15)
O1^{viii}K2N3^{x}	163.41(6)	N2N3N4	106.0(2)
O1^{viii}K2N10^{ix}	66.59(5)	N1N2K1^{iii}	114.64(15)
O1^{viii}K2N5^{x}	123.16(6)	N3N2K1^{iii}	123.85(16)
O1^{viii}K2C4^{viii}	23.28(6)	N3N2N1	111.7(2)
O3K2O4^{vii}	152.45(6)	C4N6K2	128.33(17)
O3^{ix}K2O1^{viii}	68.42(6)	C4N6C3	101.4(2)
O3K2O1^{viii}	62.74(6)	C3N6K2	129.74(17)
O3K2O3^{ix}	79.53(6)	O3N10K2^{ix}	59.14(13)
O3^{ix}K2O2^{ix}	44.25(5)	O3N10O2	120.1(2)
O3K2O2^{ix}	118.84(6)	O3N10N9	124.1(2)

O3^{ix}K2N7^{vii}	105.47(5)	O2N10K2^{ix}	62.54(13)
O3K2N7^{vii}	135.40(6)	O2N10N9	115.8(2)
O3K2N9^{viii}	78.19(6)	N9N10K2^{ix}	168.47(17)
O3^{ix}K2N9^{viii}	111.73(6)	O1N5K2^{v}	101.10(13)
O3^{ix}K2N3^{x}	100.23(6)	C3N5K2^{v}	122.49(17)
O3K2N3^{x}	128.85(6)	C3N5O1	102.11(19)
O3K2N6	59.11(6)	N4C1N7	117.5(2)
O3K2N10^{ix}	97.88(6)	N1C1N7	134.7(2)
O3^{ix}K2N10^{ix}	22.18(5)	N1C1N4	107.8(2)
O3K2N5^{x}	76.91(6)	O1C4K2^{xi}	59.97(12)
O3^{ix}K2N5^{x}	66.16(6)	O1C4N9	109.9(2)
O3^{ix}K2C4^{viii}	91.38(6)	N9C4K2^{xi}	60.18(13)
O3K2C4^{viii}	61.54(6)	N6C4K2^{xi}	145.59(18)
O2^{ix}K2O1^{viii}	73.74(6)	N6C4O1	113.1(2)
O2^{ix}K2N7^{vii}	63.53(5)	N6C4N9	136.9(2)
O2^{ix}K2N9^{viii}	99.12(6)	N6C3C2	120.1(2)
O2^{ix}K2N3^{x}	89.69(6)	N5C3N6	117.2(2)
O2^{ix}K2N10^{ix}	22.44(5)	N5C3C2	122.7(2)
O2^{ix}K2N5^{x}	95.22(6)	N4C2C3	111.7(2)
O2^{ix}K2C4^{viii}	92.72(6)	N4C2H2A	109.300
N9^{viii}K2N7^{vii}	58.51(6)	N4C2H2B	109.300
N9^{viii}K2N3^{x}	142.17(6)	C3C2H2A	109.300
H2AC2H2B	107.900	C3C2H2B	109.300

(i) x, y, -1+z; (ii) x, 1.5-y, -0.5+z; (iii) 2-x, -0.5+y, 0.5-z; (iv) 1-x, 1-y, 1-z; (v) x, 0.5-y, -0.5+z; (vi) 2-x, 0.5+y, 0.5-z; (vii) x, 1.5-y, 0.5+z; (viii) 1-x, 0.5+y, 1.5-z; (ix) 1-x, 1-y, 2-z; (x) x, 0.5-y, 0.5+z; (xi) 1-x, -0.5+y, 1.5-z.

Table S7. Composition of detonation products of compound **4**

Products	mol/mol	mol/kg	Mol %
N_2	4.97E+00	1. 826724E01	49.7377
C(d)	1.61E+00	5.92E+00	16.1292
H_2O	9.73E−01	3.57E+00	9.7330
CH_2O_2	9.43E−01	3.47E+00	9.4391
CO_2	7.19E−01	2.64E+00	7.1904
CO	7.03E−01	2.58E+00	7.0297
NH_3	1.15E−02	2.93E−02	0.101
H_2	1.03E−02	2.61E−02	0.0901
CH_4	2.08E−03	5.29E−03	0.0182
HCN	1.89E−03	4.79E−03	0.0165
C_2H_6	9.78E−05	2.48E−04	0.0009
C_2H_4	8.79E−05	2.23E−04	0.0008
CH_3OH	2.83E−05	7.17E−05	0.0002
NO	5.75E−06	1.46E−05	0.0001
N_2H_4	3.41E−06	8.66E−06	0

H	2.42E−06	6.13E−06	0
NH_2	2.34E−06	5.95E−06	0
CH_2O	9.25E−07	2.35E−06	0
OH	6.57E−07	1.67E−06	0
CHNO	5.11E−07	1.30E−06	0
CNO	5.11E−07	1.30E−06	0
O_2	2.02E−07	5.12E−07	0
O	1.02E−07	2.58E−07	0
NO_2	9.34E−09	2.37E−08	0
N_2O	8.36E−09	2.12E−08	0
N	7.47E−09	1.90E−08	0
C(gr)	2.75E−10	6.98E−10	0

Table S8. Composition of detonation products of compound **5**

Products	mol/mol	mol/kg	Mol %
N_2	5.75E+00	1.88E+01	41.4956
H_2O	3.51E+00	1.15E+01	25.3420
C(d)	2.98E+00	9.75E+00	21.5208
NH_3	4.68E−01	1.53E+00	3.3735
CH_2O_2	4.52E−01	1.47E+00	3.2558
CO	3.07E−01	1.00E+00	2.2159
H_2	1.49E−01	4.85E−01	1.0713
CO_2	1.37E−01	4.49E−01	0.9907
H_2	1.43E−02	6.59E−02	0.1879
CH_4	7.62E−03	3.52E−02	0.1005
HCN	7.46E−04	3.45E−03	0.0098
C_2H_6	5.48E−04	2.53E−03	0.0072
C_2H_4	1.53E−04	7.06E−04	0.002
CH_3OH	4.86E−05	2.24E−04	0.0006
N_2H_4	1.57E−06	7.25E−06	0
CH_2O	7.63E−07	3.53E−06	0
NH_2	7.15E−07	3.30E−06	0
H	6.67E−07	3.08E−06	0
NO	4.79E−07	2.21E−06	0
CHNO	2.30E−07	1.06E−06	0
OH	1.36E−07	6.28E−07	0
CNO	3.00E−08	1.39E−07	0
O_2	8.46E−09	3.91E−08	0
O	3.88E−09	1.79E−08	0
N_2O	5.30E−10	2.45E−09	0
C(gr)	3.71E−10	1.71E−09	0
N	2.30E−10	1.06E−09	0
NO_2	2.24E−10	1.04E−09	0
NO_2	2.24E−10	1.04E−09	0

Table S9. Composition of detonation products of compound **6**

Products	mol/mol	mol/kg	Mol %
N_2	4.97E+00	1.43E+01	51.0947
C(d)	2.15E+00	6.18E+00	22.1037
K_2CO_3(s)	1.00E+00	2.87E+00	10.2718
H_2O	7.02E−01	2.02E+00	7.2105
CO	3.68E−01	1.06E+00	3.7814
CO_2	2.58E−01	7.41E−01	2.6527
CH_2O_2	2.07E−01	5.93E−01	2.1228
NH_3	3.97E−02	1.14E−01	0.4074
H_2	1.97E−02	5.70E−02	0.2040
CH_4	1.51E−02	3.14E−02	0.0883
C_2H_6	6.26E−03	1.30E−02	0.0366
C_2H_4	7.57E−05	1.58E−04	0.0004
CH_3OH	5.54E−05	1.15E−04	0.0003
HCN	5.21E−05	1.08E−04	0.0003
N_2H_4	1.22E−06	2.54E−06	0
OH	8.88E−07	1.85E−06	0
CNO	3.89E−07	8.11E−07	0
O_2	2.44E−07	5.09E−07	0
K	5.03E−08	1.46E−07	0
C(gr)	3.92E−10	1.13E−09	0
KH	2.48E−12	7.11E−12	0
K_2CO_3	4.88E−13	1.40E−12	0
K_2O(s)	2.68E−17	7.69E−17	0

4. General methods.

All the reagents were obtained from commercial sources and used without further purification. Single-crystal X-ray diffractions were performed on a Bruker APEX-II CCD diffractometer with highly oriented graphite crystal monochromated MoK_α radiation (λ= 0.071073 nm). Semi-empirical absorption corrections were applied using SADABS program. 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 **4**, **5** and **6** are 2062977, 2062976, and 2062975. TGA measurements were carried out on a METTLER TOLEDO TGA/DSC 3+ instrument with a heating rate of 10 °C·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*) and friction sensitivity (*FS*) were measured on home-made devices according to the UN Recommendations on the Transport of Dangerous Goods, Manual of Tests and Criteria.

5. References.

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