Electronic Supplementary Information

In situ synthesized 3D metal-organic frameworks (MOFs) constructed from transition metal cations and tetrazole derivatives : a family of insensitive energetic materials

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1. Single-crystal X-ray Diffraction Analysis of Complex **1**

Table S1. Selected bond lengths [Å] of complex **1**

parameter		Length (Å)
Ag1	N1	2.2111(18)
Ag1	N3	2.262(2)
Ag1	N4	2.2595(19)
N1	N2	1.351(2)
N1	C1	1.338(3)
N3	Ag1	2.262(2)
N3	N2	1.312(3)
N3	N4	1.354(3)
N4	Ag1	2.2595(19)
N4	C1	1.328(3)
C1	C2	1.482(3)
C2	H2A	0.98
C2	H2B	0.98
C2	H2C	0.98

Table S2. Selected bond angles [^{o}] for complex **1**

parameter			bond angel (°)
N1	Ag1	N3	127.00(7)
N1	Ag1	N4	125.32(7)
N4	Ag1	N3	107.68(7)
N2	N1	Ag1	125.37(15)
C1	N1	Ag1	127.79(15)
C1	N1	N2	106.04(18)
N2	N3	Ag1	126.12(15)
N2	N3	N4	109.57(18)
N4	N3	Ag1	123.81(15)
N3	N2	N1	108.37(18)
N3	N4	Ag1	126.24(15)
C1	N4	Ag1	127.07(15)
C1	N4	N3	105.51(17)
N1	C1	C2	124.9(2)
N4	C1	N1	110.50(19)
N4	C1	C2	124.62(19)
C1	C2	H2A	109.5
C1	C2	H2B	109.5
C1	C2	H2C	109.5
H2A	C2	H2B	109.5
H2A	C2	H2C	109.5
H2B	C2	H2C	109.5

Table S3. Selected torsion angles [^{o}] of **1**

parameter				torsion angle (^{o})
Ag1	N1	N2	N3	-169.76(14)
Ag1	N1	C1	N4	169.35(14)
Ag1	N1	C1	C2	-11.1(3)
Ag1	N3	N2	N1	171.79(15)
Ag1	N3	N4	Ag1	19.3(2)
Ag1	N3	N4	C1	-172.45(15)
Ag1	N4	C1	N1	168.66(15)
Ag1	N4	C1	C2	-10.9(3)
N3	N4	C1	N1	0.5(2)
N3	N4	C1	C2	-179.0(2)
N2	N1	C1	N4	-0.7(3)
N2	N1	C1	C2	178.8(2)
N2	N3	N4	Ag1	-168.39(15)
N2	N3	N4	C1	-0.1(2)
N4	N3	N2	N1	-0.3(3)
C1	N1	N2	N3	0.6(3)

2. Single-crystal X-ray Diffraction Analysis of Complex **2**

Table S4. Selected bond lengths [Å] of complex **2**

parameter		Length (Å)
Cd01	N2	2.371(9)
Cd01	N2	2.371(9)
Cd01	N3	2.345(7)
Cd01	N3	2.345(7)
Cd01	N3	2.345(6)
Cd01	N3	2.345(6)
Cd02	N1	2.356(9)
Cd02	N1	2.356(9)
Cd02	N1	2.356(9)
Cd02	N4	2.370(10)
Cd02	N4	2.370(10)
Cd02	N4	2.370(10)
N1	N1	1.29(2)
N1	N2	1.366(13)
N2	C1	1.338(13)
N3	N4	1.338(9)
N3	C3	1.324(11)
N3	N5	1.324(11)
N4	N3	1.338(9)
C3	C3	1.32(2)
C3	C4	1.44(3)
N5	N5	1.32(2)

N5	C4	1.44(3)
C1	N2	1.338(13)
C1	C2	1.510(16)
C2	H2A	0.9598
C2	H2C	0.9609
C2	H2B	0.96
C4	H4A	0.97
C4	H4B	0.97
C4	H4C	0.97

Table S5. Selected bond angles [^{o}] for complex **2**

parameter			bond angel (°)
N2	Cd01	N2	180.00(11)
N3	Cd01	N2	91.0(2)
N3	Cd01	N2	89.0(2)
N3	Cd01	N2	89.0(2)
N3	Cd01	N2	91.0(2)
N3	Cd01	N2	89.0(2)
N3	Cd01	N2	89.0(2)
N3	Cd01	N2	91.0(2)
N3	Cd01	N2	91.0(2)
N3	Cd01	N3	88.4(4)
N3	Cd01	N3	88.4(4)
N3	Cd01	N3	180
N3	Cd01	N3	180
N3	Cd01	N3	91.6(4)
N3	Cd01	N3	91.6(4)
N1	Cd02	N1	89.7(4)
N1	Cd02	N1	89.7(4)
N1	Cd02	N1	89.7(4)
N1	Cd02	N4	90.5(2)
N1	Cd02	N4	179.7(3)
N1	Cd02	N4	90.5(2)
N1	Cd02	N4	179.7(3)
N1	Cd02	N4	90.5(2)
N1	Cd02	N4	90.5(2)
N1	Cd02	N4	90.5(2)
N1	Cd02	N4	179.7(4)
N1	Cd02	N4	90.5(2)
N4	Cd02	N4	89.3(3)
N4	Cd02	N4	89.3(3)
N4	Cd02	N4	89.3(3)
N1	N1	Cd02	125.5(2)
N1	N1	N2	109.6(6)
N2	N1	Cd02	124.9(7)

N1	N2	Cd01	124.1(7)
C1	N2	Cd01	131.1(8)
C1	N2	N1	104.8(9)
N4	N3	Cd01	124.1(6)
C3	N3	Cd01	128.7(6)
C3	N3	N4	107.2(7)
N5	N3	Cd01	128.7(6)
N5	N3	N4	107.2(7)
N3	N4	Cd02	125.9(5)
N3	N4	Cd02	125.9(5)
N3	N4	N3	108.3(9)
N3	C3	C4	130.9(13)
C3	C3	N3	108.7(5)
C3	C3	C4	120.3(11)
N3	N5	C4	130.9(13)
N5	N5	N3	108.7(5)
N5	N5	C4	120.3(11)
N2	C1	N2	111.1(13)
N2	C1	C2	124.5(6)
N2	C1	C2	124.5(6)

3. Single-crystal X-ray Diffraction Analysis of Complex **3**

Table S6. Selected bond lengths [Å] of complex **3**

parameter		Length (Å)
Pb1	N12	2.63(2)
Pb1	O1	2.32(2)
Pb1	O2	2.396(18)
Pb1	N3AA	2.55(2)
Pb3	O1	2.680(18)
Pb3	N11	2.50(2)
Pb3	O2	2.574(17)
Pb3	N6	2.55(2)
Pb3	N10	2.50(2)
Pb2	O1	2.28(2)
Pb2	O2	2.486(17)
Pb2	N0AA	2.70(2)
Pb2	N2AA	2.60(2)
N12	Pb1	2.63(2)
N12	N8	1.34(3)
N12	N11	1.36(3)
N8	N13	1.39(3)
N11	Pb3	2.50(2)
N11	C7	1.36(3)
N1	N3	1.33(3)
N1	N2	1.34(3)

N13	C7	1.32(4)
N7	N4	1.34(4)
N7	C3	1.30(3)
N4	N6	1.28(4)
O2	Pb3	2.574(17)
N3	C2	1.33(3)
N0AA	N2	1.38(3)
N0AA	C2	1.36(3)
C7	N14	1.37(4)
O3	H3A	0.8501
O3	H3B	0.8499
C3	N2AA	1.33(3)
C3	N1AA	1.37(3)
N5	N3AA	1.38(3)
N5	N9	1.25(3)
N2AA	N6	1.33(3)
N3AA	C6	1.33(3)
C6	N10	1.36(3)
C6	N14	1.38(3)
N6	Pb3	2.55(2)
N9	N10	1.40(3)
N10	Pb3	2.50(2)
N14	H14	0.86
N1AA	H1AA	0.86
N1AA	C2	1.36(3)

Table S7. Selected bond angles [^{o}] for complex **3**

parameter			bond angel (°)
O1	Pb1	N12	77.1(7)
O1	Pb1	O2	71.1(6)
O1	Pb1	N3AA	71.9(7)
O2	Pb1	N12	79.2(6)
O2	Pb1	N3AA	88.7(6)
N3AA	Pb1	N12	148.9(7)
N11	Pb3	O1	128.9(6)
N11	Pb3	O2	83.8(6)
N11	Pb3	N6	76.0(7)
O2	Pb3	O1	136.9(6)
N6	Pb3	O1	128.9(7)
N6	Pb3	O2	80.7(7)
N10	Pb3	O1	72.0(7)
N10	Pb3	N11	68.3(7)
N10	Pb3	O2	150.3(6)
N10	Pb3	N6	82.6(7)
O1	Pb2	O2	70.0(7)

O1	Pb2	N0AA	81.4(7)
O1	Pb2	N2AA	81.4(8)
O2	Pb2	N0AA	142.5(6)
O2	Pb2	N2AA	83.9(6)
N2AA	Pb2	N0AA	67.7(7)
N8	N12	Pb1	119.8(16)
N8	N12	N11	109.6(19)
N11	N12	Pb1	129.8(14)
N12	N8	N13	109(2)
Pb1	O1	Pb3	116.1(9)
Pb2	O1	Pb1	108.0(7)
Pb2	O1	Pb3	117.2(9)
N12	N11	Pb3	119.2(14)
C7	N11	Pb3	137.3(18)
C7	N11	N12	103(2)
N3	N1	N2	112(2)
C7	N13	N8	103(2)
C3	N7	N4	104(2)
N6	N4	N7	110(2)
Pb1	O2	Pb3	120.1(7)
Pb1	O2	Pb2	99.3(6)
Pb2	O2	Pb3	118.0(7)
N1	N3	C2	105(2)
N2	N0AA	Pb2	119.6(15)
C2	N0AA	Pb2	133.6(16)
C2	N0AA	N2	105(2)
N1	N2	N0AA	106(2)
N11	C7	N14	125(3)
N13	C7	N11	115(2)
N13	C7	N14	120(2)
H3A	O3	H3B	109.5
N7	C3	N2AA	112(2)
N7	C3	N1AA	120(2)
N2AA	C3	N1AA	128(2)
N9	N5	N3AA	112(2)
C3	N2AA	Pb2	136.1(17)
N6	N2AA	Pb2	119.7(17)
N6	N2AA	C3	104(2)
N5	N3AA	Pb1	105.0(14)
C6	N3AA	Pb1	146.4(18)
C6	N3AA	N5	103.9(19)
N3AA	C6	N10	112(2)
N3AA	C6	N14	125(2)
N10	C6	N14	124(2)
N4	N6	Pb3	117.9(17)
N4	N6	N2AA	110(2)
N2AA	N6	Pb3	131.7(18)
N5	N9	N10	109(2)

C6	N10	Pb3	138.1(17)
C6	N10	N9	103.4(19)
N9	N10	Pb3	117.7(15)
C7	N14	C6	126(2)
C7	N14	H14	117.2
C6	N14	H14	117.2
C3	N1AA	H1AA	115.8
C2	N1AA	C3	128(2)
C2	N1AA	H1AA	115.8
N3	C2	N0AA	112(2)
N3	C2	N1AA	123(2)
N0AA	C2	N1AA	125(2)

Table S8. Selected torsion angles [^{o}] of **3**

parameter				torsion angle (^{o})
Pb1	N12	N8	N13	169.2(15)
Pb1	N12	N11	Pb3	15(3)
Pb1	N12	N11	C7	-169(2)
Pb1	N3AA	C6	N10	-150(2)
Pb1	N3AA	C6	N14	34(5)
Pb3	N11	C7	N13	175.6(19)
Pb3	N11	C7	N14	-8(5)
Pb2	N0AA	N2	N1	-167.3(16)
Pb2	N0AA	C2	N3	163.3(18)
Pb2	N0AA	C2	N1AA	-17(4)
Pb2	N2AA	N6	Pb3	-9(3)
Pb2	N2AA	N6	N4	-179(2)
N12	N8	N13	C7	1(3)
N12	N11	C7	N13	1(3)
N12	N11	C7	N14	177(3)
N8	N12	N11	Pb3	-175.8(16)
N8	N12	N11	C7	0(3)
N8	N13	C7	N11	-1(3)
N8	N13	C7	N14	-178(3)
N11	N12	N8	N13	-1(3)
N11	C7	N14	C6	7(5)
N1	N3	C2	N0AA	1(3)
N1	N3	C2	N1AA	-178(3)
N13	C7	N14	C6	-176(3)
N7	N4	N6	Pb3	-171(2)
N7	N4	N6	N2AA	1(4)
N7	C3	N2AA	Pb2	177(2)
N7	C3	N2AA	N6	-4(3)
N7	C3	N1AA	C2	-173(3)
N4	N7	C3	N2AA	4(4)

N4	N7	C3	N1AA	179(3)
N3	N1	N2	N0AA	2(3)
N2	N1	N3	C2	-2(3)
N2	N0AA	C2	N3	0(3)
N2	N0AA	C2	N1AA	180(3)
C3	N7	N4	N6	-3(4)
C3	N2AA	N6	Pb3	171.8(18)
C3	N2AA	N6	N4	2(3)
C3	N1AA	C2	N3	-174(3)
C3	N1AA	C2	N0AA	7(5)
N5	N3AA	C6	N10	-1(3)
N5	N3AA	C6	N14	-177(2)
N5	N9	N10	Pb3	-168.2(18)
N5	N9	N10	C6	3(3)
N2AA	C3	N1AA	C2	1(5)
N3AA	N5	N9	N10	-4(3)
N3AA	C6	N10	Pb3	167.5(18)
N3AA	C6	N10	N9	-1(3)
N3AA	C6	N14	C7	180(3)
N9	N5	N3AA	Pb1	166(2)
N9	N5	N3AA	C6	3(3)
N10	C6	N14	C7	4(4)
N14	C6	N10	Pb3	-16(4)
N14	C6	N10	N9	175(2)
N1AA	C3	N2AA	Pb2	3(5)
N1AA	C3	N2AA	N6	-178(3)
C2	N0AA	N2	N1	-1(3)

Table S9. Hydrogen bonds of **3**

Donor	--H	....Acceptor	D – H (Å)	H...A (Å)	D...A (Å)	D - H...A (°)
N1AA	--H1AA	..N8	0.86	2.01	2.86(3)	171
O3	--H3A	..N4	0.84	2.56	2.96(4)	111
O3	--H3B	..N3AA	0.85	2.27	3.08(4)	158
O3	--H3B	..N5	0.85	2.34	3.15(4)	159
O3	--H3B	..N9	0.85	2.51	3.26(4)	148
N14	--H14	..N1	0.86	2.07	2.93(3)	176

4. Single-crystal X-ray Diffraction Analysis of Complex **4**

Table S10. Selected bond lengths [Å] of complex **4**

parameter		Length (Å)
Pb1	N6	2.668(15)
Pb1	N6	2.668(15)
Pb1	N4	2.805(14)

Pb1	N1	2.723(13)
Pb1	N1	2.723(13)
C1	C1	1.4550(8)
C1	N6	1.37(2)
C1	N4	1.30(2)
N3	C2	1.40(2)
N3	N2	1.307(18)
C4	N6	1.41(2)
C4	N5	1.32(2)
N6	Pb1	2.668(15)
N4	N5	1.375(18)
C9	N1	1.273(18)
C9	N2	1.272(18)
C2	C2	1.35(3)
C2	N1	1.41(2)

Table S11. Selected bond angles [^{o}] for complex **4**

parameter			bond angel (°)
N6	Pb1	N6	65.4(6)
N6	Pb1	N4	150.8(5)
N6	Pb1	N4	124.2(4)
N6	Pb1	N1	81.3(4)
N6	Pb1	N1	81.3(4)
N6	Pb1	N1	81.1(5)
N6	Pb1	N1	81.1(5)
N1	Pb1	N4	125.8(4)
N1	Pb1	N4	74.1(4)
N1	Pb1	N1	159.0(6)
N6	C1	C1	121.2(7)
N4	C1	C1	124.4(8)
N4	C1	N6	114.3(9)
N2	N3	C2	103.4(13)
N5	C4	N6	108.7(14)
C1	N6	Pb1	116.1(9)
C1	N6	C4	101.8(13)
C4	N6	Pb1	142.1(11)
C1	N4	Pb1	114.1(9)
C1	N4	N5	104.8(12)
N5	N4	Pb1	141.1(10)
N2	C9	N1	114.6(13)
C4	N5	N4	110.2(13)
N3	C2	N1	107.8(13)
C2	C2	N3	125(3)
C2	C2	N1	126(3)
C9	N1	Pb1	144.7(10)

C9	N1	C2	102.7(13)
C2	N1	Pb1	112.1(10)
C9	N2	N3	111.2(13)

5. IR Spectra of **1**-**4**

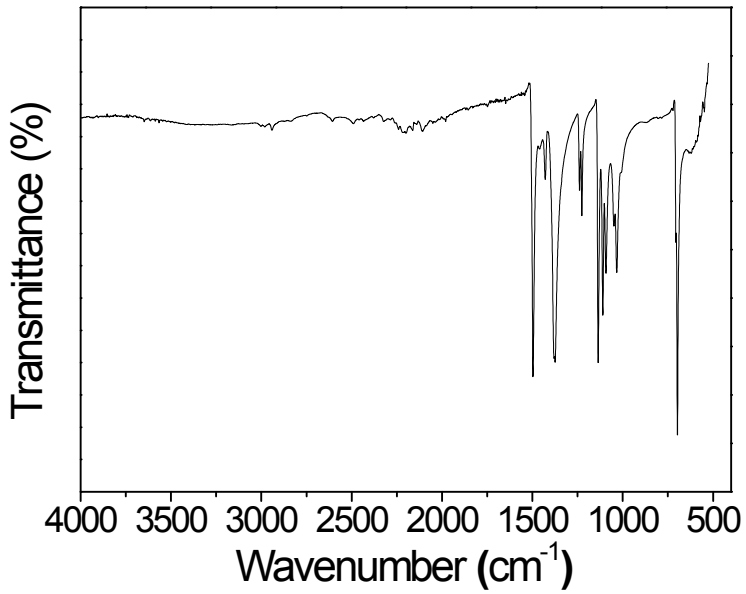

Fig. S1 IR spectrum of **1**

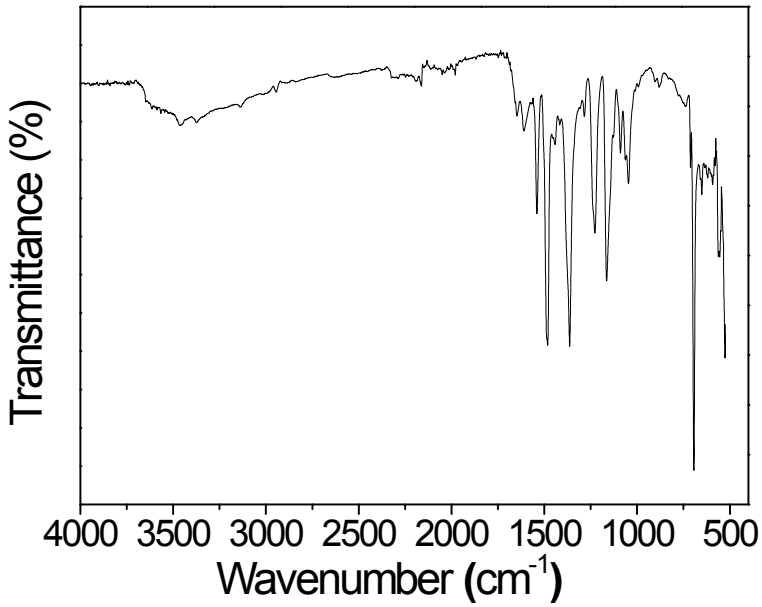

Fig. S2 IR spectrum of **2**

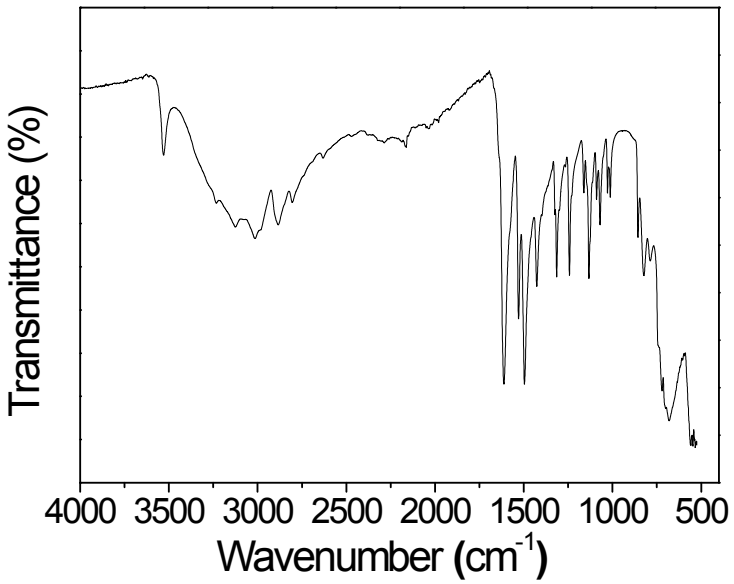

Fig. S3 IR spectrum of **3**

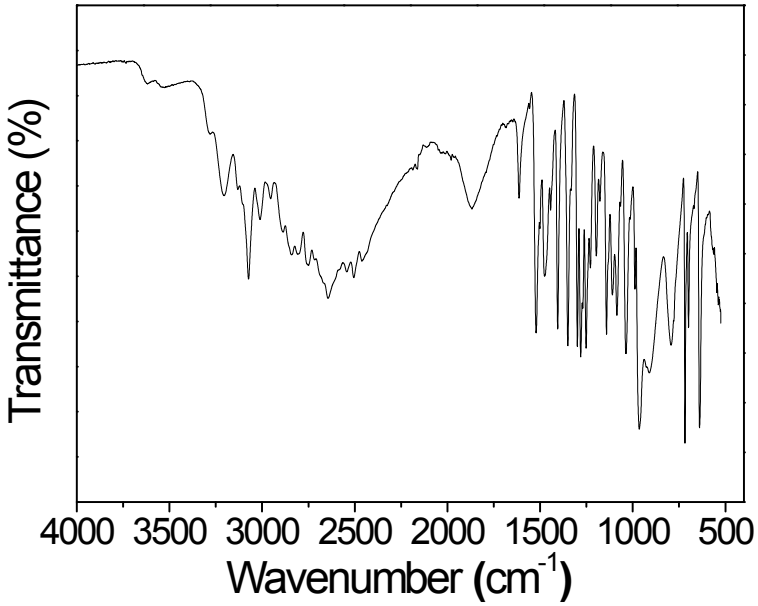

Fig. S4 IR spectrum of **4**

6. Powder X-ray Diffraction of Complexes **1**-**4**

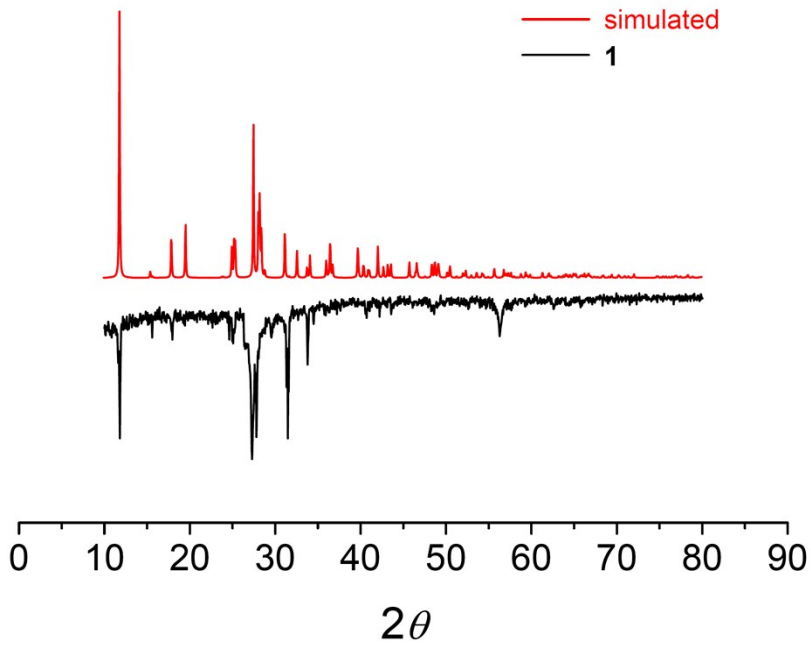

Fig. S5 Powder X-ray diffraction pattern of **1** (black) and the calculated pattern (red) from the single crystal structure of **1**

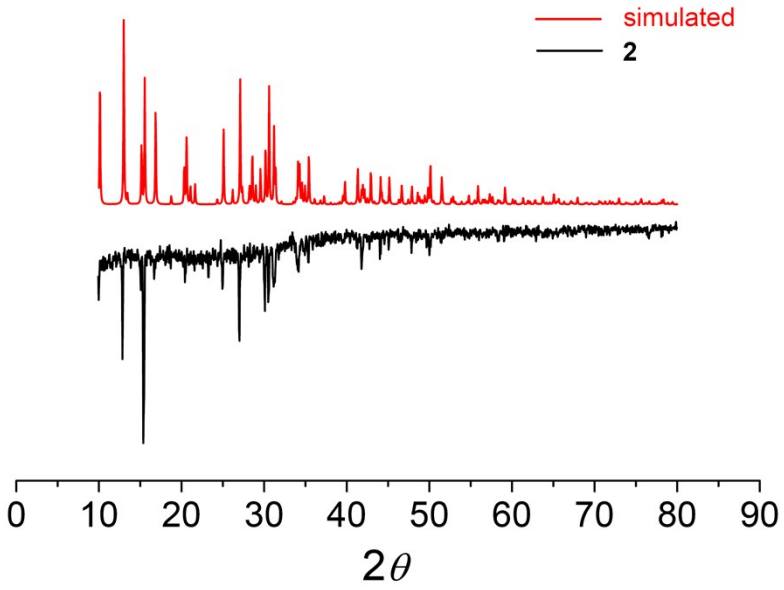

Fig. S6 Powder X-ray diffraction pattern of **2** (black) and the calculated pattern (red) from the single crystal structure of **2**

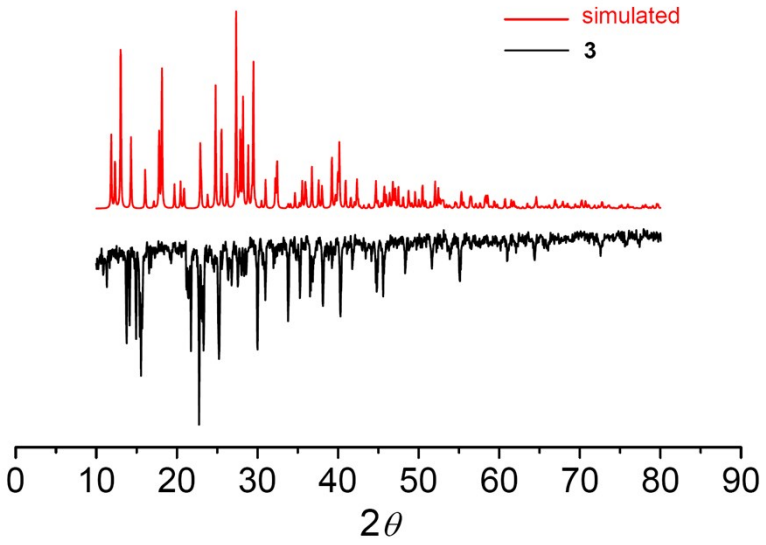

Fig. S7 Powder X-ray diffraction pattern of **3** (black) and the calculated pattern (red) from the single crystal structure of **3**

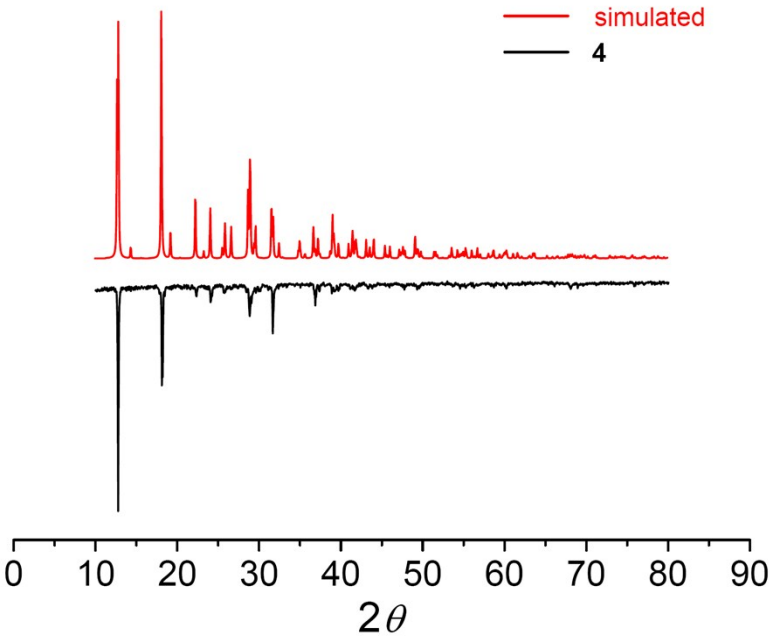

Fig. S8 Powder X-ray diffraction pattern of **4** (black) and the calculated pattern (red) from the single crystal structure of **4**

7. Computational details

The experimental results for the constant volume combustion energies ($\Delta_c U$) of the EMOFs **1**-**4** are -7541.167 J g^{-1}, -9832.833 J g^{-1}, -2239.167 J g^{-1}, and -8495.933 J g^{-1}, respectively. According to the formula $\Delta_c H_m^\theta = \Delta_c U_m^\theta + \Delta nRT, \Delta n = n_g(products) - n_g(reactants)$, ($n_g$ is the total molar amount of gases in the products or reactants, R = 8.314 J mol^{-1} K^{-1}, and T = 298.15 K), the enthalpies of combustion $(\Delta_c H_m^\theta)$ can be derived to be -1437.46 kJ mol^{-1} for eqn (1), -12856.04 kJ mol^{-1} for eqn (2), -2160.60 kJ mol^{-1} for eqn (3), and -4193.88 kJ mol^{-1} for eqn (4), respectively. The combustion reaction equations are listed as follows:

$$AgC_2H_3N_4(s) + 3O_2(g) \rightarrow \frac{1}{2}Ag_2O(s) + 2CO_2(g) + \frac{3}{2}H_2O(l) + 2N_2(g) \quad (1)$$

$$Cd_5C_{18}H_{27}N_{36}(s) + \frac{109}{4}O_2(g) \rightarrow 5CdO(s) + 18CO_2(g) + \frac{27}{2}H_2O(l) + 18N_2(g) \quad (2)$$

$$Pb_3C_4H_4N_{18}O_3(s) + 5O_2(g) \rightarrow 3PbO(s) + 4CO_2(g) + 2H_2O(l) + 9N_2(g) \quad (3)$$

$$Pb_2C_{12}H_8N_{28}O_2(s) + 14O_2(g) \rightarrow 2PbO(s) + 12CO_2(g) + 4H_2O(l) + 14N_2(g) \quad (4)$$

$$\Delta_f H_m^\theta(1,s) = \frac{1}{2}\Delta_f H_m^\theta(Ag_2O, s) + 2\Delta_f H_m^\theta(CO_2, g) + \frac{3}{2}\Delta_f H_m^\theta(H_2O, l) - \Delta_c H_m^\theta(1, s) \quad (5)$$

$$\Delta_f H_m^\theta(2,s) = 5\Delta_f H_m^\theta(CdO, s) + 18\Delta_f H_m^\theta(CO_2, g) + \frac{27}{2}\Delta_f H_m^\theta(H_2O, l) - \Delta_c H_m^\theta(2, s) \quad (6)$$

$$\Delta_f H_m^\theta(3,s) = 3\Delta_f H_m^\theta(PbO, s) + 4\Delta_f H_m^\theta(CO_2, g) + 2\Delta_f H_m^\theta(H_2O, l) - \Delta_c H_m^\theta(3, s) \quad (7)$$

$$\Delta_f H_m^\theta(4,s) = 2\Delta_f H_m^\theta(PbO, s) + 12\Delta_f H_m^\theta(CO_2, g) + 4\Delta_f H_m^\theta(H_2O, l) - \Delta_c H_m^\theta(4, s) \quad (8)$$

Based on the calculated enthalpies of combustion and the known enthalpies of formation of the combustion products[1] determined experimentally, Ag_2O(s), $\Delta_c H_m^\theta$(Ag_2O, s) = -31 kJ mol^{-1}, CdO(s), $\Delta_c H_m^\theta$(CdO, s) = (-258.35 ± 0.40) kJ mol^{-1}, PbO(s), $\Delta_c H_m^\theta$(PbO, s) = (-219.50 ± 0.27) kJ mol^{-1}, CO_2(g), $\Delta_c H_m^\theta$(CO_2, g) = (-393.51 ± 0.13) kJ mol^{-1}, H_2O (l), $\Delta_c H_m^\theta$(H_2O, l) = (-285.830 ± 0.04) kJ mol^{-1}, the standard enthalpies of formation of

EMOFs **1-4**, $\Delta_c H_m^\theta$, were back-calculated from the combustion equations. On the basis of Hess's law in thermochemical eqn (5) - (8), the standard enthalpies of formation ($\Delta_f H_m^\theta$) of **1-4** are calculated to be (206.20 ± 0.32) kJ mol^{-1}, (622.40 ± 4.88) kJ mol^{-1}, (-643.60 ± 1.41) kJ mol^{-1}, and (1041.66 ± 2.26) kJ mol^{-1}, respectively.

On the basis of the largest exothermic principle proposed by Kamlet-Jacobs (K-J),[2] We employed a widely used empirical method[3,4,5] which employed the hypothesis of BKW equation and arbitrary theory of the Kamlet-Jacobs method to investigate the detonation properties of metal-containing explosives. For systems with metals, the most stable products of detonation reaction were assumed under the constraints of stoichiometrically available oxygen.[6] The detonation reactions of **1-4** are described by equation (9) - (12), and the detonation properties are calculated by
K-J equations as follows:

$$AgC_2H_3N_4(s) \rightarrow Ag(s) + 2C(s) + NH_3(g) + \frac{3}{2}N_2(g) \quad (9)$$

$$Cd_5C_{18}H_{27}N_{36}(s) \rightarrow 5Cd(s) + 18C(s) + 9NH_3(g) + \frac{27}{2}N_2(g) \quad (10)$$

$$Pb_3C_4H_4N_{18}O_3(s) \rightarrow 3Pb(s) + \frac{7}{2}C(s) + 2H_2O(g) + \frac{1}{2}CO_2(g) + 9N_2(g) \quad (11)$$

$$Pb_2C_{12}H_8N_{28}O_2(s) \rightarrow 2Pb(s) + 12C(s) + 2H_2O(g) + \frac{4}{3}NH_3(g) + \frac{40}{3}N_2(g) \quad (12)$$

$$D = 1.01\varphi^{\frac{1}{2}}(1 + 1.30\rho)$$

$$P = 1.558\varphi\rho^2$$

$$\varphi = 31.68N(MQ)^{1/2}$$

$$Q = \frac{-[\Delta_f H_m^\theta(detonation\ products) - \Delta_f H_m^\theta(explosive)]}{formula\ weight\ of\ explosive}$$

where: D is detonation velocity (km s^{-1}), P is detonation pressure (GPa), N is moles of detonation gases per gram of explosive, M is average molecular weight of the gases, Q is the chemical energy of detonation (kcal g^{-1}) and ρ is the density of explosive (g cm^{-3}).

According to the known enthalpies of formation, including NH_3(g) (-46 kJ mol^{-1}), H_2O(g) (-242 kJ mol^{-1}), CO_2(g) (-393 kJ mol^{-1}) and the $\Delta_f H_m^\theta$ of **1**-**4**, the Q for **1**-**4** are 0.316, 0.189, 0.009, and 0.634 kcal·g^{-1}, respectively. Utilizing the above equations (9-12), and the known values of N, M and Q, the D and P can be obtained (Table S12).

Table S12. The D and P values and the parameters associated with them

	Q_v J g^{-1}	$\Delta_c H_m$ kJ mol^{-1}	$\Delta_f H_m$ kJ mol^{-1}	N mol g^{-1}	M g mol^{-1}	Q kcal g^{-1}	φ	ρ g cm^{-3}	D km s^{-1}	P GPa
1	-7541.167	-1437.46	206.20	0.0131	23.6202	0.316	1.133	2.995	5.260	15.83
2	-9832.833	-12856.04	622.40	0.0172	23.6202	0.189	1.150	2.137	4.093	8.18
3	-2239.167	-2160.60	-643.60	0.0118	26.9697	0.009	0.185	4.144	2.774	4.95
4	-8495.933	-4193.88	1041.66	0.0168	25.9347	0.634	2.161	2.486	6.283	20.81

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