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Two new energetic coordination compounds based on Tetrazole-1-acetic acid: Syntheses, crystal structures and their synergistic catalytic effect for thermal decomposition of ammonium perchlorate

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Fig.S1. Experimental and simulated powder XRD patterns of compounds 1(a) and 2(b).

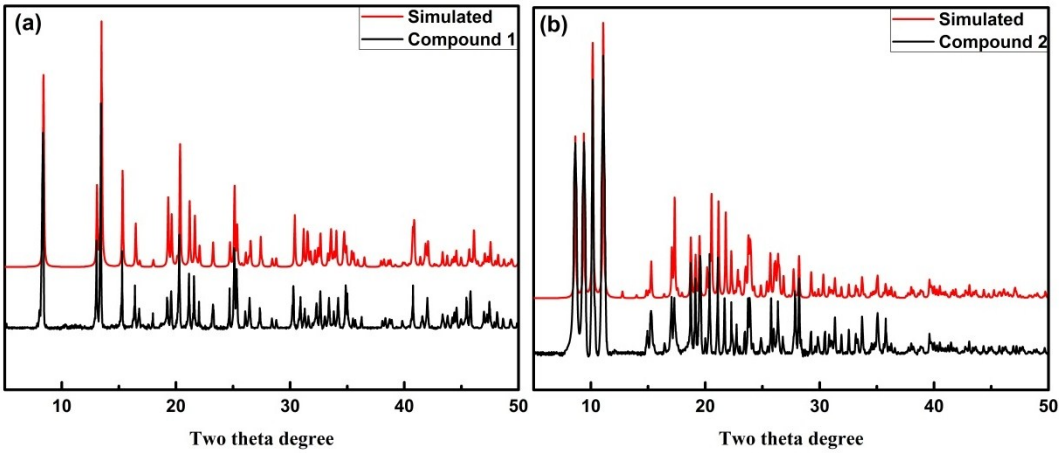

Table S1Crystal data and structure refinement for coordination compounds **1** and **2**

Compound	1	2
Empirical formula	$C_5 H_7 Bi N_4 O_8$	$C_{18} H_{24} Fe_3 N_{25} O_{19}$
Formula weight	460.13	1060.16
Temperature	293(2) K	293(2) K
Wavelength	0.71073 Å	0.71073 Å
Crystal system	Orthorhombic	Monoclinic
Space group	*Pbca*	*C2/c*

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a(Å)	8.8215(8)	12.0154(13)
b(Å)	11.1197(10)	20.745(2)
c(Å)	21.054(2)	16.311(2)
α（°）	90	90
β（°）	90	102.087(3)
γ（°）	90	90
V(Å^3)	2065.2(3)	3975.4(8)
Z	8	4
ρ(cald.)(Mg/m^3)	2.960	1.771
μ(mm^{-1})	17.122	1.187
F(000)	2730	2140
Theta range for data collection(°)	3.01 to 27.56	1.96 to 27.54
h/*k*/*l*	-11≤*h*≤11,-13≤*k*≤14, -27≤*l*≤22	-15≤h≤15,-22≤k≤26, -21≤l≤21
Reflections collected / unique	18500 / 2381 [R(int) = 0.0586]	18716 / 4565 [R(int) = 0.0469]
Completeness to theta = 27.56	99.6 %	99.4 %
Data/restraints/parameters	2381 / 3 / 183	4565 / 0 / 293
Goodness-of-fit on F^2	1.054	1.107
Final *R* indices [I>2σ(I)]	R_1 =0.0327, wR_2 = 0.0805	R_1 = 0.0499, wR_2 = 0.1373
R indices (all data)	R_1=0.0.0404, wR_2 =0.0.0846	R1 = 0.0767, wR2 = 0.1597
Largest diff. peak and hole(e.A^{-3})	2.015 and -2.538	1.027 and -1.002

Table S2 Selected Bond Distances (Å) and Angles (°) for coordination compounds 1 and 2

Compound 1			
Bi(1)-O(5)	2.362(4)	Bi(1)-O(1W)	2.558(4)
Bi(1)-O(1)	2.399(4)	Bi(1)-O(4)i	2.604(4)

Bi(1)-O(6)	2.475(4)	Bi(1)-O(2)	2.648(4)
Bi(1)-O(3)i	2.505(4)	Bi(1)-O(6)iii	2.670(3)
Bi(1)-N(2)ii	2.551(5)		
N(2)ii-Bi(1)-O(6)iii	142.19(14)	O(6)-Bi(1)-O(3) i	108.38(12)
O(1W)-Bi(1)-O(6)iii	81.67(13)	O(5)-Bi(1)-N(2)ii	77.95(14)
O(4)i-Bi(1)-O(6)iii	71.78(12)	O(1)-Bi(1)-N(2)ii	77.23(15)
O(2)-Bi(1)-O(6)iii	70.77(13)	O(6)-Bi(1)-N(2)ii	142.39(14)
O(5)-Bi(1)-O(1)	75.15(14)	O(3)i-Bi(1)-N(2)ii	71.62(13)
O(5)-Bi(1)-O(6)	67.82(11)	O(5)-Bi(1)-O(1W)	145.40(14)
O(1)-Bi(1)-O(6)	79.31(14)	O(1)-Bi(1)-O(1W)	122.49(14)
O(5)-Bi(1)-O(3)i	69.30(16)	O(6)-Bi(1)-O(1W)	139.68(14)
O(1)-Bi(1)-O(3) i	136.50(14)	O(3)i-Bi(1)-O(1W)	79.75(14)
O(4)i-Bi(1)-O(2)	132.21(12)	N(2)ii-Bi(1)-O(1W)	77.93(15)
O(5)-Bi(1)-O(6)iii	131.51(13)	O(5)-Bi(1)-O(4)i	104.36(14)
O(1)-Bi(1)-O(6)iii	87.65(14)	O(1)-Bi(1)-O(4)i	152.21(14)
O(6)-Bi(1)-O(6)iii	64.53(12)	O(6)-Bi(1)-O(4)i	75.07(16)
O(3)i-Bi(1)-O(6)iii	134.99(13)	O(3)i-Bi(1)-O(4)i	63.78(11)
O(4)i-Bi(1)-O(2)	132.21(12)	N(2)ii-Bi(1)-O(4)i	130.33(14)
O(5)-Bi(1)-O(6)iii	131.51(13)	O(1W)-Bi(1)-O(4)i	73.85(15)
O(3)i-Bi(1)-O(2)	138.42(12)	O(5)-Bi(1)-O(2)	122.61(13)
N(2)ii-Bi(1)-O(2)	72.83(14)	O(1)-Bi(1)-O(2)	50.98(13)
O(1W)-Bi(1)-O(2)	72.32(13)	O(6)-Bi(1)-O(2)	112.89(12)

Symmetry transformations used to generate equivalent atoms: i: x+1/2,-y+3/2,-z； ii -x+2,y+1/2,-z+1/2； iii -x+2,-y+1,-z；

Compound 2

O(7)-Fe(1)	2.018(3)	Fe(1)-O(4)	2.058(3)
O(8)-Fe(1)	1.898(3)	Fe(2)-O(2)	1.997(3)

O(8) -Fe(2) i	1.9216(16)	Fe(2)-O(9)	2.006(3)
O(8)-Fe(2)	1.9216(16)	Fe(2)-O(1)i	2.007(3)
Fe(1)-O(6)i	2.041(2)	Fe(2)-O(3)	2.014(3)
Fe(1)-O(6)	2.041(2)	Fe(2)-O(5)	2.023(2)
Fe(1)-O(4)i	2.058(3)	O(1)-Fe(2)i	2.007(3)
Fe(1)-O(8)-Fe(2)i	120.61(8)	O(8)-Fe(2)-O(1)i	93.37(10)
Fe(1)-O(8)-Fe(2)	120.61(8)	O(2)-Fe(2)-O(1)i	91.00(13)
Fe(2)i-O(8)-Fe(2)	118.79(15)	O(9)-Fe(2)-O(1)i	83.57(12)
O(8)-Fe(1)-O(7)	180.000(1)	O(8)-Fe(2)-O(3)	92.89(9)
O(8)-Fe(1)-O(6)i	97.14(7)	O(2)-Fe(2)-O(3)	169.32(11)
O(7)-Fe(1)-O(6)i	82.86(7)	O(9)-Fe(2)-O(3)	84.42(12)
O(8)-Fe(1)-O(6)	97.14(7)	O(1)i-Fe(2)-O(3)	91.28(13)
O(7)-Fe(1)-O(6)	82.86(7)	O(8)-Fe(2)-O(5)	96.71(9)
O(6)i-Fe(1)-O(6)	165.71(14)	O(2)-Fe(2)-O(5)	89.59(12)
O(8)-Fe(1)-O(4)i	91.83(7)	O(9)-Fe(2)-O(5)	86.27(12)
O(7)-Fe(1)-O(4)i	88.17(7)	O(1)i-Fe(2)-O(5)	169.75(11)
O(6)i-Fe(1)-O(4)i	91.78(11)	O(6)i-Fe(1)-O(4)	87.77(11)
O(6)-Fe(1)-O(4)i	87.77(11)	O(6)-Fe(1)-O(4)	91.78(11)
O(8)-Fe(1)-O(4)	91.83(7)	O(4)i-Fe(1)-O(4)	176.34(14)
O(7)-Fe(1)-O(4)	88.17(7)	O(8)-Fe(2)-O(2)	97.40(10)
O(2)-Fe(2)-O(9)	85.47(12)	O(8)-Fe(2)-O(9)	175.86(11)

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

Table S3 Hydrogen bond interactions in **2**

D-H···A	D···A(Å)
O9-H5···N8	2.735
O7-H2···N4	2.748
O9-H6···N11	2.666