Two novel lead(II)-tetrazolate frameworks based on cubane $[Pb_4(OH)_4]^{4+}$ clusters trapping long lifetime luminescence emission

Jiayin Sun,[a] Daojun Zhang,[b] Li Wang,[a] Yu Cao,[a] Da Li,[a] Liying Zhang,[a] Wei Song,[a] Yong Fan*[a] and Jianing Xu*[a]

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Table S1 Selected bond lengths (Å) and angles (º) for compounds **1** and **2**.

Compound **1**

N(1)-Pb(4)$^{\#1}$	2.688(8)	O(2)-Pb(3)	2.417(7)
N(3)-Pb(1)	2.697(9)	O(2)-Pb(2)	2.504(6)
N(4)-Pb(2)	2.727(8)	O(3)-Pb(3)	2.330(7)
N(11)-Pb(3)	2.721(9)	O(3)-Pb(4)	2.418(7)
N(12)-Pb(1)	2.729(9)	O(3)-Pb(1)	2.449(6)
O(1)-Pb(4)	2.352(7)	O(4)-Pb(2)	2.338(7)
O(1)-Pb(2)	2.384(7)	O(4)-Pb(3)	2.353(6)
O(1)-Pb(1)	2.431(7)	O(4)-Pb(1)	2.513(7)
O(2)-Pb(4)	2.322(8)	Pb(4)-N(1)$^{\#2}$	2.688(8)
O(1)-Pb(1)-O(3)	71.0(2)	O(1)-Pb(2)-N(4)	74.0(3)
O(1)-Pb(1)-O(4)	67.9(2)	O(2)-Pb(2)-N(4)	137.0(3)
O(3)-Pb(1)-O(4)	68.7(2)	O(3)-Pb(3)-O(4)	73.5(2)
O(1)-Pb(1)-N(3)	82.0(3)	O(3)-Pb(3)-O(2)	72.2(3)
O(3)-Pb(1)-N(3)	135.1(3)	O(4)-Pb(3)-O(2)	71.5(2)
O(4)-Pb(1)-N(3)	68.0(3)	O(3)-Pb(3)-N(11)	75.7(3)
O(1)-Pb(1)-N(12)	137.0(3)	O(4)-Pb(3)-N(11)	77.1(2)
O(3)-Pb(1)-N(12)	81.3(2)	O(2)-Pb(3)-N(11)	140.0(3)
O(4)-Pb(1)-N(12)	71.7(3)	O(2)-Pb(4)-O(1)	73.8(2)
N(3)-Pb(1)-N(12)	96.2(3)	O(2)-Pb(4)-O(3)	72.3(3)
O(4)-Pb(2)-O(1)	71.6(2)	O(1)-Pb(4)-O(3)	72.9(2)
O(4)-Pb(2)-O(2)	70.2(2)	O(2)-Pb(4)-N(1)$^{\#2}$	87.5(3)

O(1)-Pb(2)-O(2)	70.0(2)	O(1)-Pb(4)-N(1)$^{\#2}$	70.9(2)
O(4)-Pb(2)-N(4)	76.9(2)	O(3)-Pb(4)-N(1)$^{\#2}$	142.3(2)
Compound **2**			
Pb(1)-O(1)$^{\#1}$	2.327(9)	Pb(1)-Pb(1)$^{\#1}$	3.8172(11)
Pb(1)-O(1)	2.398(12)	Pb(1)-Pb(1)$^{\#3}$	3.9170(9)
Pb(1)-O(1)$^{\#2}$	2.512(9)	O(1)-Pb(1)$^{\#2}$	2.327(9)
Pb(1)-N(1)	2.660(13)	O(1)-Pb(1)$^{\#1}$	2.512(8)
Pb(1)-O(2)	2.820(8)	O(2)-Pb(1)$^{\#4}$	2.820(8)
Pb(1)-Pb(1)$^{\#2}$	3.8172(11)	N(5)-Pb(1)$^{\#4}$	3.000(10)
O(1)$^{\#1}$-Pb(1)-O(1)	73.4(4)	O(1)-Pb(1)-O(2)	144.7(3)
O(1)$^{\#1}$-Pb(1)-O(1)$^{\#2}$	70.1(4)	O(1)$^{\#2}$-Pb(1)-O(2)	112.6(4)
O(1)-Pb(1)-O(1)$^{\#2}$	70.2(4)	N(1)-Pb(1)-O(2)	85.5(4)
O(1)$^{\#1}$-Pb(1)-N(1)	82.3(4)	Pb(1)$^{\#2}$-O(1)-Pb(1)	107.8(4)
O(1)-Pb(1)-N(1)	75.2(4)	Pb(1)$^{\#2}$-O(1)-Pb(1)$^{\#1}$	108.0(4)
O(1)$^{\#2}$-Pb(1)-N(1)	140.4(4)	Pb(1)-O(1)-Pb(1)$^{\#1}$	102.0(4)
O(1)$^{\#1}$-Pb(1)-O(2)	75.0(4)	Pb(1)$^{\#4}$-O(2)-Pb(1)	110.6(4)

Symmetry transformations used to generate equivalent atoms for **1**: #1 -x+1/2, y, z-1/2 #2 -x+1/2, y, z+1/2. For **2**: #1 -y, x, -z+3/2 #2 y, -x, -z+3/2 #3 -x, -y, z #4 x, y, -z+1 #5 -y+1/2, -x+1/2, -z+3/2 #6 y+1/2, x-1/2, -z+3/2 #7 -x, -y-1, -z+1.

Table S2 Bond lengths (Å) and angles (º) of hydrogen bonds for compounds **2**.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(2)-H(10B)...N(4)$^{\#8}$	0.97	2.59	3.50(2)	157.2
O(2)-H(10B)...N(3)$^{\#8}$	0.97	1.71	2.68(2)	175.2
O(2)-H(10A)...N(5)$^{\#9}$	0.97	2.60	3.41(2)	141.6
O(2)-H(10A)...N(6)$^{\#9}$	0.97	1.89	2.85(2)	172.4

Symmetry transformations used to generate equivalent atoms: #1 -y, x, -z+3/2 #2 y, -x, -z+3/2 #3 -x, -y, z #4 x, y, -z+1 #5 -y+1/2, -x+1/2, -z+3/2 #6 y+1/2, x-1/2, -z+3/2 #7 -x, -y-1, -z+1 #8 -x+1/2, y+1/2, z #9 -x, -y, -z+1.

Table S3 Factors influenced the synthesis for compound **1** and **2**.

Run	*n*Pb(Ac): *n*H_2BDT	V(H_2O) mL	Temperature ℃	Reaction time/d	pH	Results
1	3:1	3	160	2	5.1	Complex **1+2**
2	3:2	3	160	2	5.1	Complex **1**
3	3:3	3	160	2	5.1	Complex **1+2**
4	3:2	3	140	2	5.1	Complex **1**
5	3:2	3	180	2	5.1	Complex **1**
6	3:2	3	160	5	5.1	Complex **1+2**
7	3:2	5~11	160	2	5.1	Complex **1+2**
8	3:2	13	160	2	5.04	Complex **2**
9	3:2	3	160	2	4.8	amorphous
10	3:2	3	160	2	6	amorphous
11	3:2	3	160	2	6.5	amorphous
12	3:2	3	160	2	7	amorphous

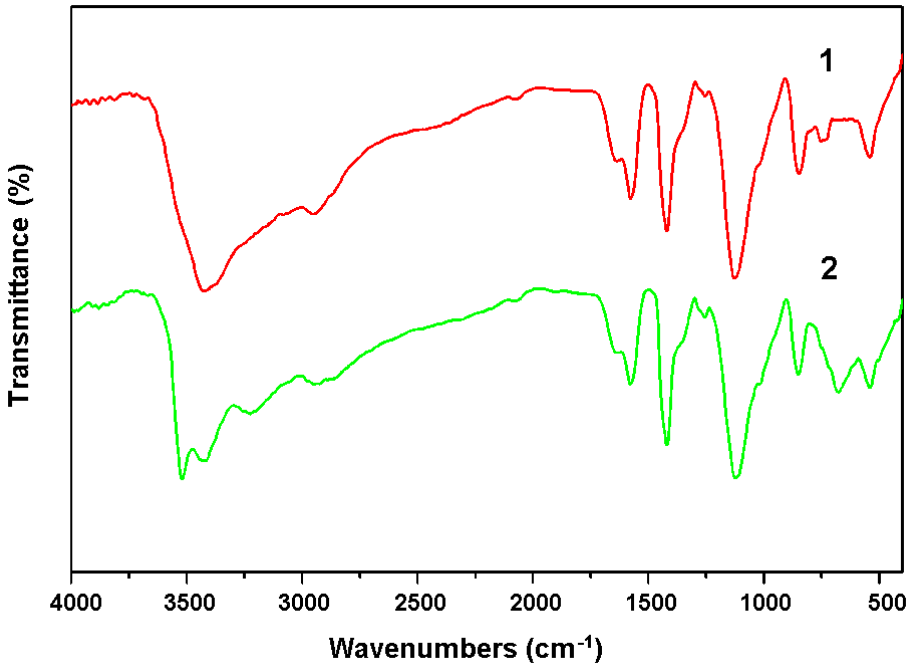

Fig. S1 IR Spectra of compound **1** and **2**.

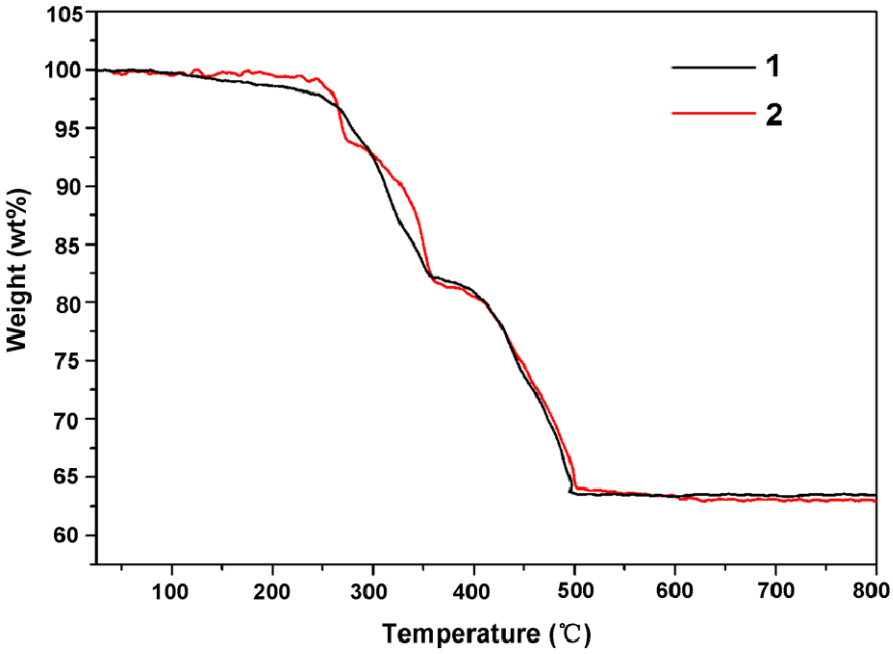

Fig. S2 The TGA curve of compound **1** and **2** measured under flowing air.

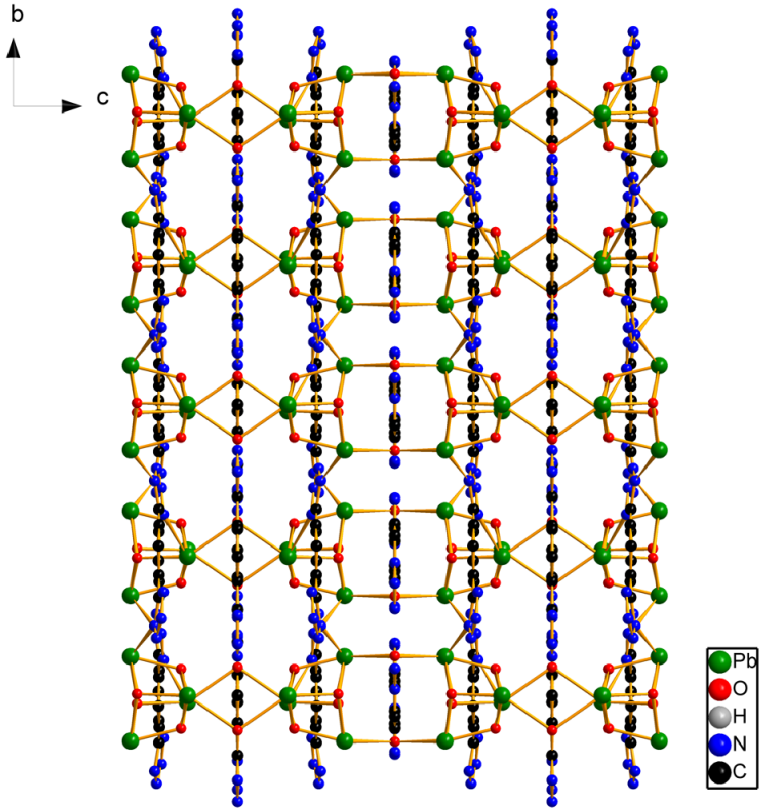

Fig. S3 3D network representation of complex **2** in *bc* plane.

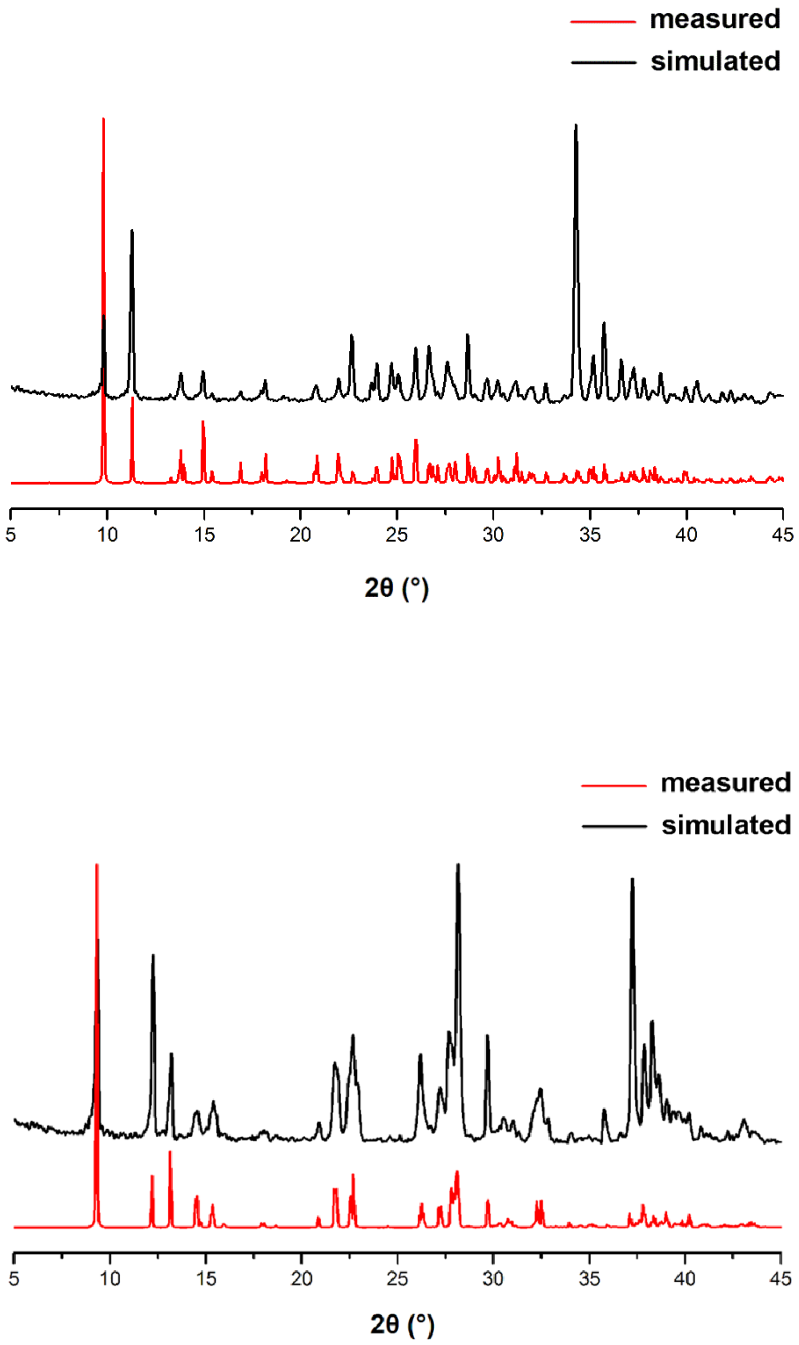

Fig. S4 Simulated and experimental X-ray diffraction patterns of compounds **1** (top) and **2** (bottom).