Electronic Supplementary Material (ESI) for CrystEngComm

Supporting Information

Rationally Designed and Syntheses of Different Series of d-f Heterometallic Coordination Frameworks Based on 1-H-benzimidazole-5-carboxylate acid

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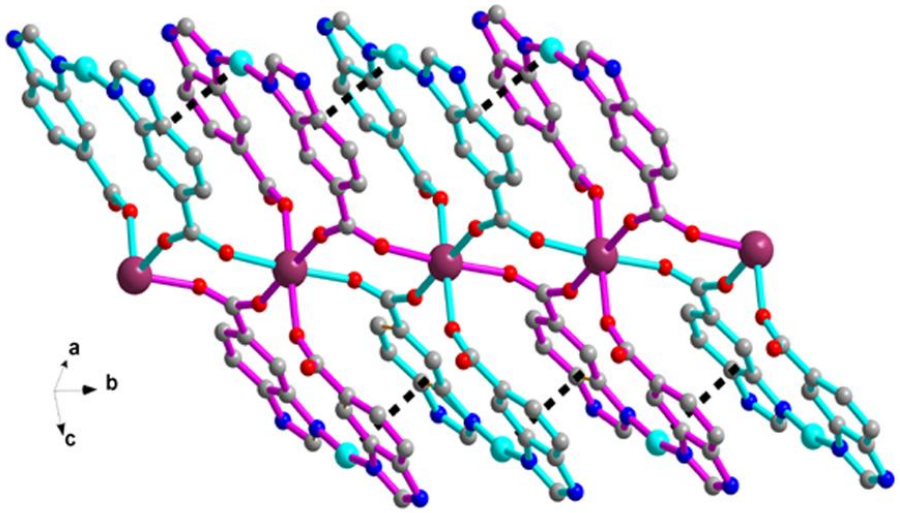

Fig. S1. The shortest distance between the Cu(I) ion and the benzimidazol ring.

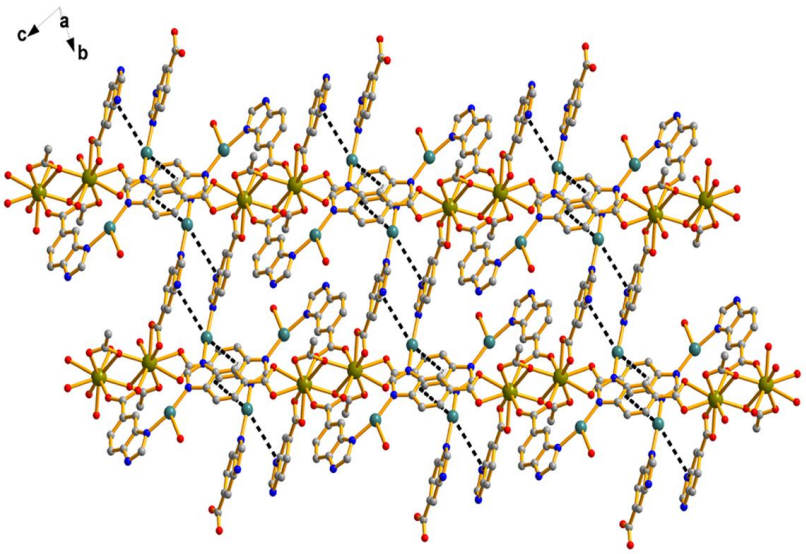

Fig. S2. The Ag2 ions interact with their neighboring benzimidazol groups in the zigzag chain with the distances in the range.

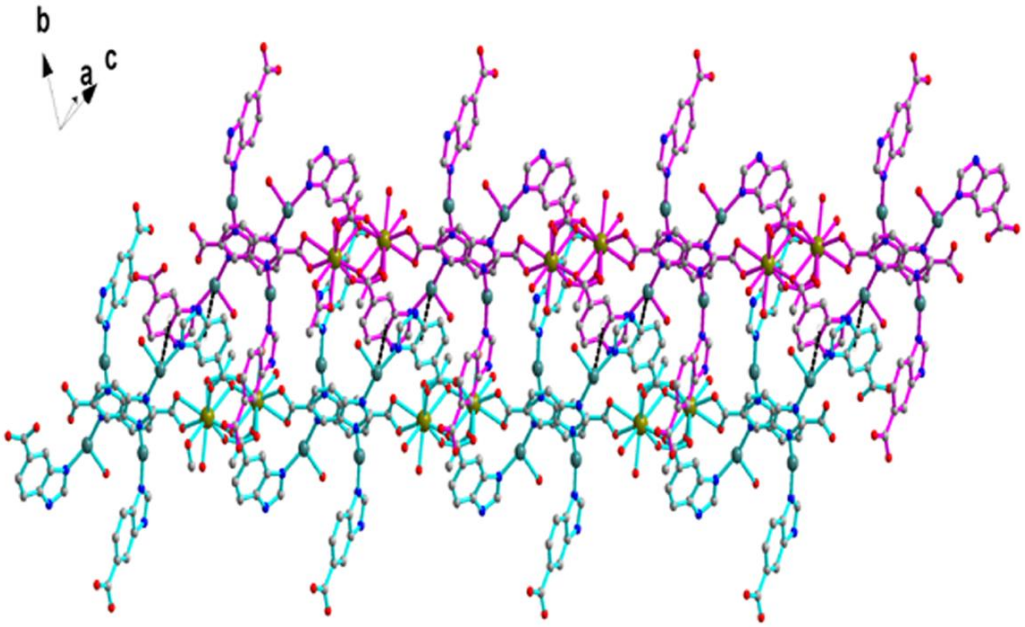

Fig. S3. Ag1 ions also interact with neighboring benzimidazol groups between these layers with the distance.

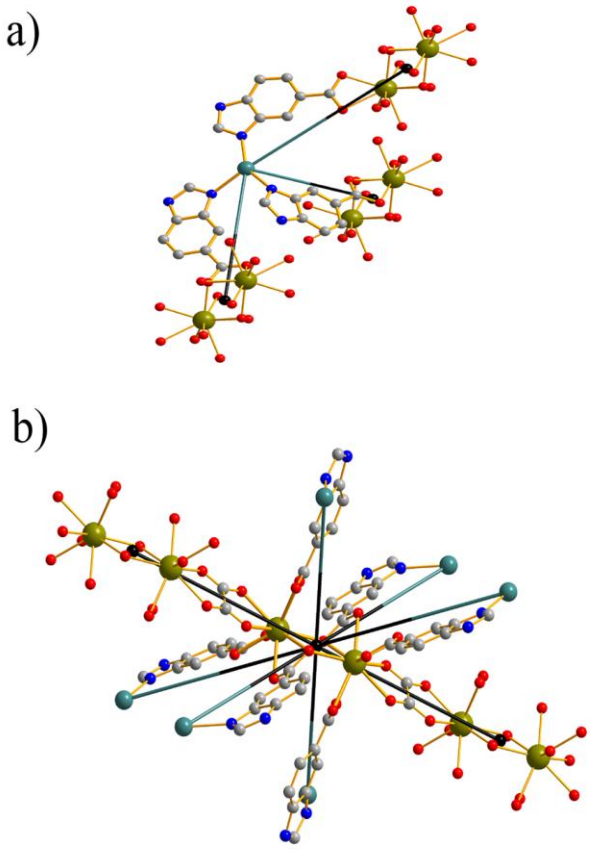

Fig. S4. (a) The 3-connected Ag node. (b) The 8-connected node simplified by dinuclear Tb subunits.

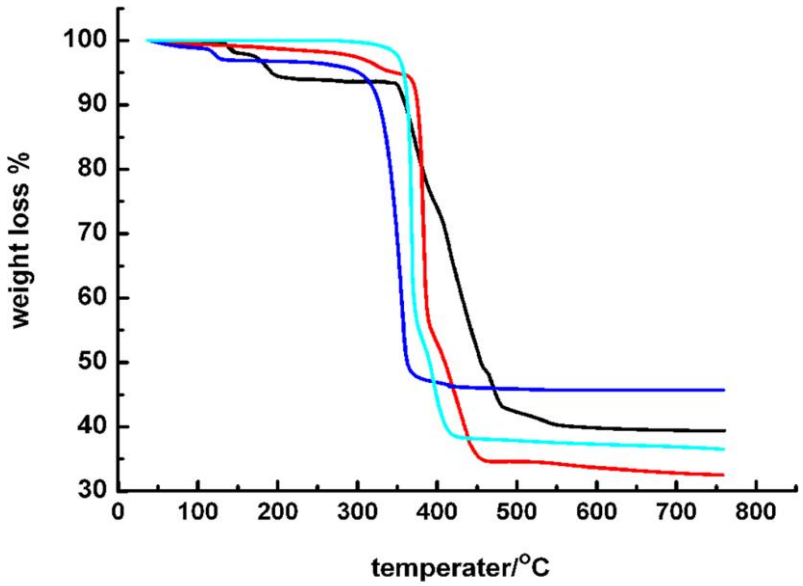

Fig. S5. The TGA curves of compound **1** (black), **3** (red), **4** (blue), **5** (cyan).

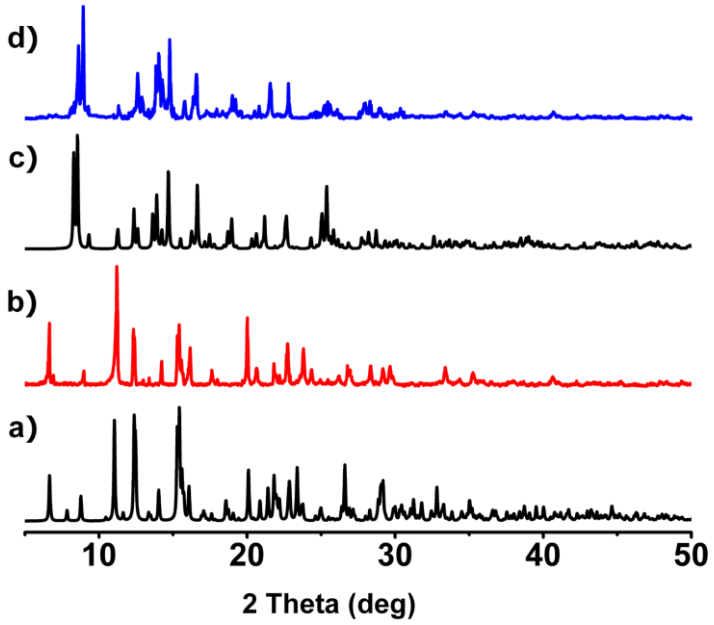

Fig. S6. The PXRD patterns (a) simulated based on the X-ray single-crystal diffraction date of **4**, (b) for as-synthesized **4**, (c) simulated based on X-ray single-crystal diffraction date of **5**, and (d) for as-synthesized **5**.

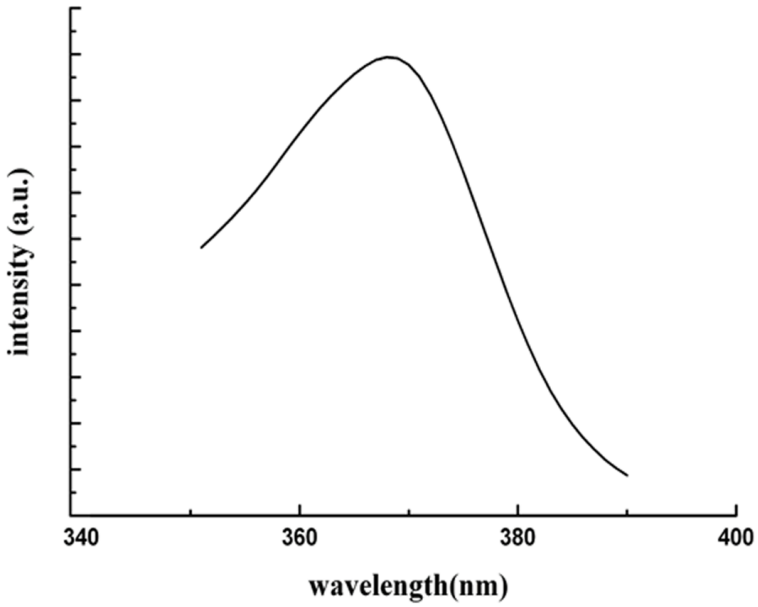

Fig. S7. Solid-state emission spectrum of H_2bic at room temperature (exited at 213 nm).

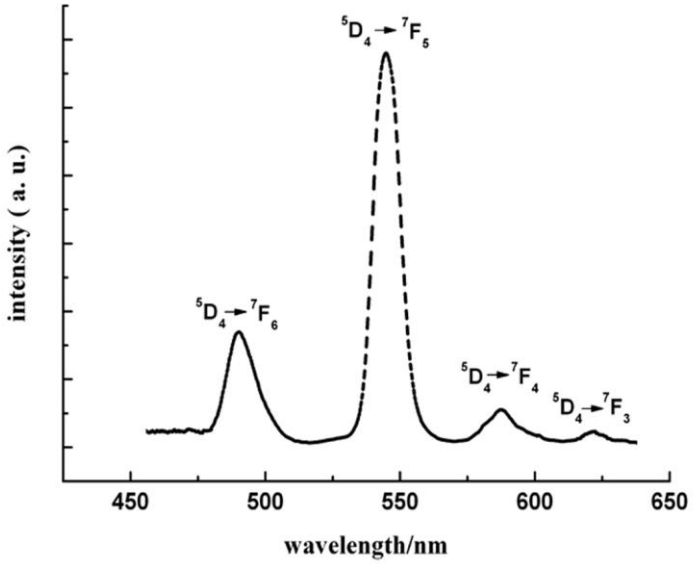

Fig. S8. Solid-state emission spectrum of 5 (a, exited at 311 nm) at room temperature.

Table S1 Selected Bond angles (°) for complexes **1**-**5**. Symmetry transformations used to generate equivalent atoms are given as footnotes.

Complex 1 [a]			
O(3)-Tb(1)-O(3)#1	180.00(15)	O(2)#3-Tb(1)-O(4)	94.40(16)
O(3)-Tb(1)-O(2)#2	87.38(17)	O(3)-Tb(1)-O(4)#1	94.30(17)
O(3)#1-Tb(1)-O(2)#2	92.62(17)	O(3)#1-Tb(1)-O(4)#1	85.70(17)
O(3)-Tb(1)-O(2)#3	92.62(17)	O(2)#2-Tb(1)-O(4)#1	94.40(16)
O(3)#1-Tb(1)-O(2)#3	87.38(17)	O(2)#3-Tb(1)-O(4)#1	85.60(16)
O(2)#2-Tb(1)-O(2)#3	179.999(1)	O(4)-Tb(1)-O(4)#1	180.00(19)
O(3)-Tb(1)-O(4)	85.70(17)	N(1)-Ag(1)-N(3)#3	170.05(19)
O(3)#1-Tb(1)-O(4)	94.30(17)	N(4)#4-Ag(2)-N(4)	180.0(3)
O(2)#2-Tb(1)-O(4)	85.60(16)		
Complex 2 [b]			
N(8)-Cu(1)-N(1)	164.4(2)	O(1)#2-Er(1)-O(2)	94.51(16)
N(8)-Cu(1)-Br(1)#1	96.85(18)	O(7)-Er(1)-O(6)#3	87.03(19)
N(1)-Cu(1)-Br(1)#1	98.53(17)	O(3)-Er(1)-O(6)#3	96.90(19)
N(5)-Cu(2)-N(4)	164.0(2)	O(1)#2-Er(1)-O(6)#3	175.8(2)
N(5)-Cu(2)-Br(1)	96.54(17)	O(2)-Er(1)-O(6)#3	88.6(2)
N(4)-Cu(2)-Br(1)	99.35(18)	O(7)-Er(1)-O(5)	93.81(19)
O(7)-Er(1)-O(3)	174.39(17)	O(3)-Er(1)-O(5)	90.12(19)
O(7)-Er(1)-O(1)#2	90.42(19)	O(1)#2-Er(1)-O(5)	85.7(2)
O(3)-Er(1)-O(1)#2	85.89(18)	O(2)-Er(1)-O(5)	179.3(2)

O(7)-Er(1)-O(2)	86.89(19)	O(6)#3-Er(1)-O(5)	91.21(16)
O(3)-Er(1)-O(2)	89.19(19)	Cu(1)#4-Br(1)-Cu(2)	167.43(4)
Complex 3 [c]			
N(1)-Cu(1)-N(8)	164.2(3)	O(1)#2-Yb(1)-O(5)	86.6(3)
N(1)-Cu(1)-Br(1)#1	98.83(19)	O(3)-Yb(1)-O(2)	89.3(2)
N(8)-Cu(1)-Br(1)#1	96.66(19)	O(7)-Yb(1)-O(2)	87.3(2)
N(5)-Cu(2)-N(4)	163.6(3)	O(1)#2-Yb(1)-O(2)	94.09(19)
N(5)-Cu(2)-Br(1)	96.58(19)	O(5)-Yb(1)-O(2)	179.3(3)
N(4)-Cu(2)-Br(1)	99.6(2)	O(3)-Yb(1)-O(6)#3	95.7(2)
O(3)-Yb(1)-O(7)	175.7(2)	O(7)-Yb(1)-O(6)#3	86.6(2)
O(3)-Yb(1)-O(1)#2	86.8(2)	O(1)#2-Yb(1)-O(6)#3	176.9(3)
O(7)-Yb(1)-O(1)#2	91.0(2)	O(5)-Yb(1)-O(6)#3	91.67(19)
O(3)-Yb(1)-O(5)	90.5(2)	O(2)-Yb(1)-O(6)#3	87.7(3)
O(7)-Yb(1)-O(5)	93.0(2)	Cu(1)#4-Br(1)-Cu(2)	168.95(5)
Complex 4 [d]			
O(1)-Eu(1)-O(8)#1	74.44(14)	O(6)-Eu(1)-O(8)	123.79(15)
O(1)-Eu(1)-O(2)#1	137.98(14)	O(4)-Eu(1)-O(8)	137.86(14)
O(8)#1-Eu(1)-O(2)#1	74.95(14)	O(7)-Eu(1)-O(8)	51.12(15)
O(1)-Eu(1)-O(6)	132.36(13)	O(1)-Eu(1)-O(3)	84.76(16)
O(8)#1-Eu(1)-O(6)	149.42(15)	O(8)#1-Eu(1)-O(3)	89.99(17)
O(2)#1-Eu(1)-O(6)	86.46(13)	O(2)#1-Eu(1)-O(3)	123.22(15)
O(1)-Eu(1)-O(4)	127.24(17)	O(6)-Eu(1)-O(3)	80.02(17)
O(8)#1-Eu(1)-O(4)	77.58(16)	O(4)-Eu(1)-O(3)	51.33(16)
O(2)#1-Eu(1)-O(4)	71.92(16)	O(7)-Eu(1)-O(3)	144.53(17)
O(6)-Eu(1)-O(4)	73.61(17)	O(8)-Eu(1)-O(3)	154.61(15)
O(1)-Eu(1)-O(7)	93.85(19)	O(1)-Eu(1)-O(5)	81.11(13)
O(8)#1-Eu(1)-O(7)	123.85(16)	O(8)#1-Eu(1)-O(5)	150.73(14)
O(2)#1-Eu(1)-O(7)	80.11(18)	O(2)#1-Eu(1)-O(5)	134.16(13)
O(6)-Eu(1)-O(7)	74.92(17)	O(6)-Eu(1)-O(5)	51.26(12)
O(4)-Eu(1)-O(7)	138.69(19)	O(4)-Eu(1)-O(5)	105.89(15)
O(1)-Eu(1)-O(8)	72.56(14)	O(7)-Eu(1)-O(5)	73.01(16)
O(8)#1-Eu(1)-O(8)	73.31(16)	O(8)-Eu(1)-O(5)	114.46(14)
O(2)#1-Eu(1)-O(8)	71.54(14)	O(3)-Eu(1)-O(5)	71.75(16)
N(6)#2-Ag(1)-N(1)	158.8(2)	N(5)#3-Ag(2)-N(4)	162.1(2)
Complex 5 [e]			
N(5)-Ag(1)-N(2)#1	145.5(3)	O(8)#1-Tb(1)-O(5)	78.6(2)
N(5)-Ag(1)-N(4)#2	112.0(3)	O(7)-Tb(1)-O(5)	71.7(2)
N(2)#1-Ag(1)-N(4)#2	102.3(3)	O(2)-Tb(1)-O(5)	145.6(2)
O(6)-Tb(1)-O(3)#3	80.68(19)	O(4)-Tb(1)-O(5)	73.34(19)
O(6)-Tb(1)-O(8)#1	128.11(19)	O(6)-Tb(1)-O(1)	82.72(19)
O(3)#3-Tb(1)-O(8)#1	149.29(19)	O(3)#3-Tb(1)-O(1)	72.02(18)
O(6)-Tb(1)-O(7)	77.4(2)	O(8)#1-Tb(1)-O(1)	117.19(19)
O(3)#3-Tb(1)-O(7)	137.60(19)	O(7)-Tb(1)-O(1)	69.56(19)
O(8)#1-Tb(1)-O(7)	67.99(19)	O(2)-Tb(1)-O(1)	52.60(18)

O(6)-Tb(1)-O(2)	134.3(2)	O(4)-Tb(1)-O(1)	158.88(18)
O(3)#3-Tb(1)-O(2)	92.4(2)	O(5)-Tb(1)-O(1)	126.64(18)
O(8)#1-Tb(1)-O(2)	75.0(2)	O(6)-Tb(1)-O(3)	143.5(2)
O(7)-Tb(1)-O(2)	78.2(2)	O(3)#3-Tb(1)-O(3)	70.6(2)
O(6)-Tb(1)-O(4)	109.1(2)	O(8)#1-Tb(1)-O(3)	78.75(17)
O(3)#3-Tb(1)-O(4)	92.19(19)	O(7)-Tb(1)-O(3)	139.10(18)
O(8)#1-Tb(1)-O(4)	69.9(2)	O(2)-Tb(1)-O(3)	70.48(19)
O(7)-Tb(1)-O(4)	129.19(19)	O(4)-Tb(1)-O(3)	51.92(17)
O(2)-Tb(1)-O(4)	116.29(18)	O(5)-Tb(1)-O(3)	125.06(19)
O(6)-Tb(1)-O(5)	53.84(19)	O(1)-Tb(1)-O(3)	108.25(17)
O(3)#3-Tb(1)-O(5)	121.1(2)		

[a] #1: -x+1,-y+1,-z+1; #2: -x+1,-y,-z+1; #3: x,y+1,z; #4: -x,-y-1,-z+1; [b] #1: x,y,z+1; #2: x,y+1,z; #3: x,y-1,z; #4: x,y,z-1; [c] #1: x,y,z-1; #2: x,y-1,z; #3: x,y+1,z; #4: x,y,z+1; [d] #1: -x+1,-y,-z+2; #2: -x,-y+1,-z+1; #3: x,y-1,z; #4: x,y+1,z; [e] #1: -x+1,-y+2,-z; #2: -x+1,-y+3,-z; #3: -x,-y+2,-z.