Supporting Information

Metal-controlled structural variations of coordination architectures constructed from the flexible 1*H*-benzimidazole-1-propionic acid

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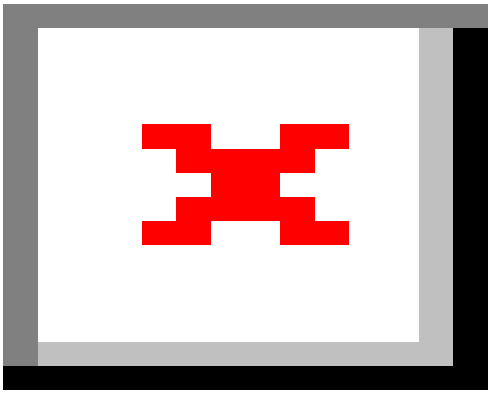
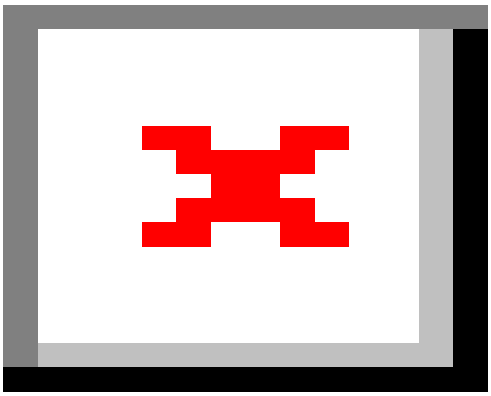
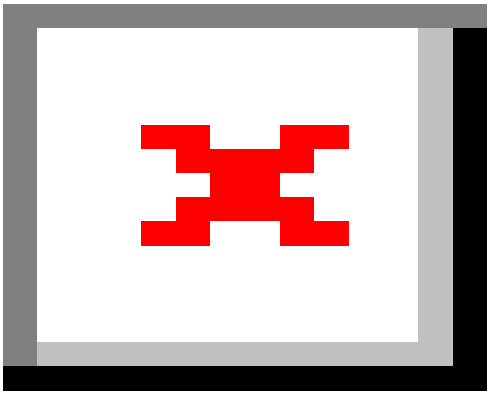
Fig.S1 Simulated and experimental powder X-ray diffraction (PXRD) patterns of complexes **1**–**6**: (a) for **1**, (b) for **2**, (c) for **3**, (d) for **4**, (e) for **5** and (f) for **6**.



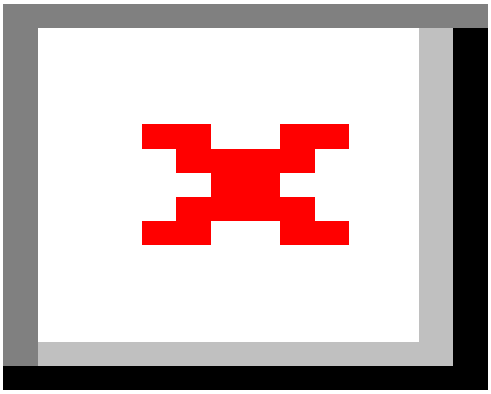
(a)



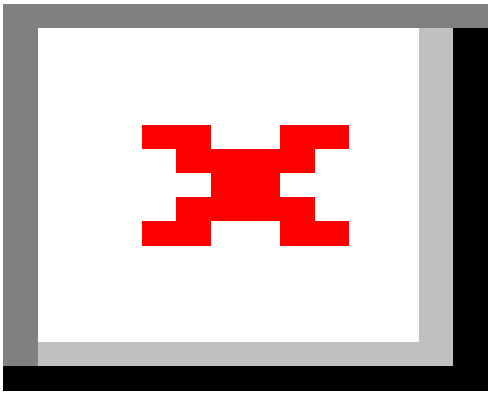
(b)



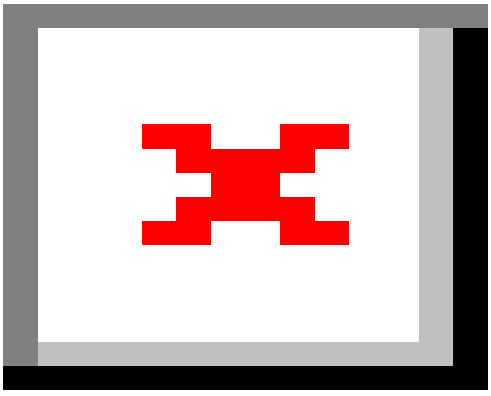
(c)



(d)



(e)



(f)

Fig.S2 TGA curves for complexes **1**–**5**.

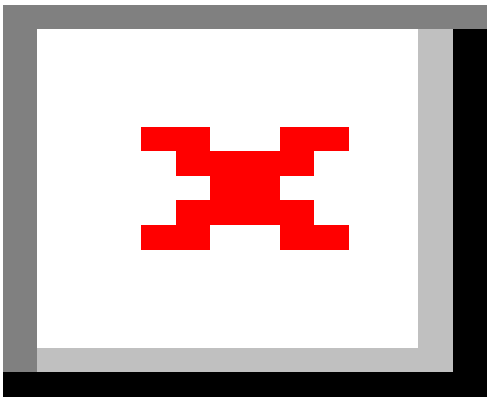


Fig.S3 The normalized solid-state photoluminescent excitation spectra of ligand Hbiap and complexes **3**–**6** at room temperature.

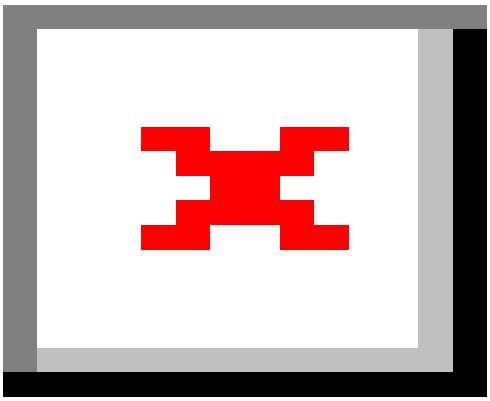


Table S1 Selected bond lengths (Å) and angles (°) for complexes **1**–**6**.

Complex **1**			
Co1–N2	2.034(3)	Co1–N4	2.039(3)
Co1–O5	1.974(2)	Co1–O7#1	1.991(2)
Co2–N6	2.045(3)	Co2–N8	2.045(3)
Co2–O1	1.954(3)	Co2–O3#2	1.932(2)
N2–Co1–N4	103.01(11)	N2–Co1–O5	116.65(11)
N2–Co1–O7#1	103.96(10)	N4–Co1–O5	110.71(11)
N4–Co1–O7#1	117.58(10)	O5–Co1–O7#1	105.26(11)
N6–Co2–N8	114.13(12)	N6–Co2–O1	111.97(11)
N6–Co2–O3#2	109.11(11)	N8–Co2–O1	102.29(11)
N8–Co2–O3#2	111.95(11)	O1–Co2–O3#2	107.06(11)
Complex **2**			
Cu1–N2	2.001(2)	Cu1–N4#1	2.011(2)
Cu1–O3	1.985(2)	Cu1–O5	1.975(2)
Cu1–O9	2.409(2)	Cu2–N6	1.998(2)
Cu2–N8	1.996(2)	Cu2–O1	1.947(2)
Cu2–O8#2	1.952(2)		
N2–Cu1–N4#1	170.15(8)	N2–Cu1–O3	89.24(8)
N2–Cu1–O5	90.04(8)	N2–Cu1–O9	95.73(8)
O3–Cu1–N4#1	87.61(7)	O5–Cu1–N4#1	92.43(7)
O9–Cu1–N4#1	93.89(7)	O3–Cu1–O5	175.88(7)
O3–Cu1–O9	96.28(7)	O5–Cu1–O9	87.83(7)
N6–Cu2–N8	179.28(9)	N6–Cu2–O1	89.74(8)
N6–Cu2–O8#2	89.75(8)	N8–Cu2–O1	90.60(8)
N8–Cu2–O8#2	89.92(8)	O1–Cu2–O8#2	179.30(8)
Complex **3**			
Ag1–N2	2.359(8)	Ag1–N2#1	1.969(6)
O2–H2C	1.23	N2–Ag1–N2#1	154.47(12)
Complex **4**			
Zn1–N2	2.035(2)	Zn1–N4	2.033(2)
Zn1–O1#1	1.954(2)	Zn1–O3#2	1.955(2)
N2–Zn1–N4	107.89(7)	N2–Zn1–O1#1	112.76(7)
N2–Zn1–O3#2	109.92(7)	N4–Zn1–O1#1	117.97(7)
N4–Zn1–O3#2	100.76(7)	O1A–Zn1–O3#2	106.72(7)
Complex **5**			
Cd1–N2	2.257(3)	Cd1–N4	2.292(3)
Cd1–O5	2.415(2)	Cd1–O6	2.322(2)
Cd1–O7	2.452(2)	Cd1–O8	2.315(2)

Cd2–N6	2.258(3)	Cd2–N8	2.243(3)
Cd2–O1	2.515(2)	Cd2–O2#1	2.294(3)
Cd2–O3	2.368(3)	Cd2–O4	2.383(2)
N2–Cd1–N4	97.04(10)	N2–Cd1–O5	98.51(10)
N2–Cd1–O6	109.67(9)	N2–Cd1–O7	85.98(9)
N2–Cd1–O8	137.19(9)	N4–Cd1–O5	141.06(9)
N4–Cd1–O6	86.36(9)	N4–Cd1–O7	99.15(9)
N4–Cd1–O8	104.97(9)	O5–Cd1–O6	54.78(8)
O5–Cd1–O7	117.35(8)	O5–Cd1–O8	86.96(8)
O6–Cd1–O7	162.77(9)	O6–Cd1–O8	107.98(9)
O7–Cd1–O8	54.86(8)	N6–Cd2–N8	111.49(11)
N6–Cd2–O1	107.89(9)	N6–Cd2–O2#1	91.82(10)
N6–Cd2–O3	137.87(10)	N6–Cd2–O4	84.28(10)
N8–Cd2–O1	82.86(10)	N8–Cd2–O2#1	134.67(10)
N8–Cd2–O3	90.10(10)	N8–Cd2–O4	107.90(10)
O1–Cd2–O2#1	52.51(9)	O1–Cd2–O3	110.46(9)
O1–Cd2–O4	160.00(9)	O3–Cd2–O2#1	97.84(9)
O3–Cd2–O4	54.17(9)	O4–Cd2–O2#1	112.84(9)
Complex **6**			
Hg1–Cl1	2.611(2)	Hg1–N2	2.163(3)
Hg2–Cl1	2.985(2)	Hg2–Cl2	2.340(2)
Cl1–Hg1–Cl1#1	100.17(7)	Cl1–Hg1–N2	102.95(10)
Cl1–Hg1–N2#1	98.87(10)	N2–Hg1–N2#1	145.72(12)
Cl1–Hg2–Cl2	90.64(4)	Cl1–Hg2–Cl2#2	89.37(4)
Cl1–Hg2–Cl1#2	180.00	Cl2–Hg2–Cl2#2	180.00

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

Table S2 Hydrogen bond distances (Å) and angles (º) for complexes **2**, **3** and **6**.

D–H···A	*d*(D–H)	*d*(H···A)	*d*(D···A)	∠D–H···A
Complex **2**				
O9–H9D···O4	0.85	2.03	2.727(3)	138
O10–H10C···O9#1	0.85	2.51	2.943(3)	112
O10–H10C···O10#1	0.85	2.53	3.249(4)	143
O10–H10D···O5	0.85	2.08	2.924(3)	174
O11–H11C···O6	0.85	1.90	2.745(3)	172
O11–H11D···O13	0.85	2.03	2.863(3)	164
O12–H12C···O2	0.85	2.15	2.812(3)	135
O12–H12D···O11	0.85	2.01	2.780(4)	151
O13–H13C···O14	0.85	1.87	2.714(3)	172
O13–H13D···O3	0.85	2.04	2.857(3)	160
O14–H14C···O8#2	0.85	2.08	2.785(3)	140
O15–H15D···O7#3	0.85	2.18	2.816(4)	131
O16–H16C···O1	0.85	1.92	2.758(3)	170
O16–H16D···O16#3	0.85	2.20	2.731(4)	120
Complex **3**				
O3–H3C···O2#1	0.85	2.47	2.919(10)	114
O3–H3D···O1#2	0.85	2.08	2.864(10)	154
Complex **6**[d]				
O2–H2C···O1#1	0.85	2.05	2.677(6)	130

Symmetry transformations used to generate equivalent atoms for **2**: #1 1–*x*, 1–*y*, 1–*z*; #2 –*x*, –*y*, 1–*z*; #3 –*x*, 1–*y*, 1–*z*. for **3**: #1 1/2–*x*, –1/2+*y*, 1/2–*z*; #2 1/2+*x*, 1/2–*y*, 1/2+*z*. for **6**: #1 –*x*, 1–*y*, –*z*.