Two pairs of isomorphism and two 3D metal-organic frameworks based on a star-like ligand tri(4-pyridylphenyl)amine

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Table S1. Selected bond lengths (Å) and angles (deg) for compounds **1-6**.

Compound **1**			
Cd(1)-O(1)	2.310(2)	Cd(1)-O(2)	2.558(2)
Cd(1)-N(2)	2.345(3)	Cd(1)-N(3)	2.505(4)
O(1)-Cd(1)-O(1)	99.97(12)	O(1)-Cd(1)-N(2)	95.89(10)
O(1)-Cd(1)-N(3)	130.01(6)	N(2)-Cd(1)-N(3)	83.13(6)
N(2)-Cd(1)-N(2)	166.25(12)	O(1)-Cd(1)-O(2)	53.13(8)
O(2)-Cd(1)-N(2)	87.98(9)	O(2)-Cd(1)-N(3)	76.93(6)
O(2)-Cd(1)-O(2)	153.86(11)		
Compound **2**			
Zn(1)-O(1)	2.112(5)	Zn(1)-O(2)	2.359(5)
Zn(1)-O(3)	2.013(4)	Zn(1)-N(1)	2.082(4)
Zn(1)-N(2)	2.067(4)	O(3)-Zn(1)-N(2)	105.57(19)
O(3)-Zn(1)-N(1)	97.31(18)	N(2)-Zn(1)-N(1)	104.32(18)
O(3)-Zn(1)-O(1)	105.35(19)	N(2)-Zn(1)-O(1)	140.59(19)
N(1)-Zn(1)-O(1)	95.33(18)	O(3)-Zn(1)-O(2)	156.63(18)
N(2)-Zn(1)-O(2)	87.97(18)	N(1)-Zn(1)-O(2)	97.61(17)
Compound **3**			
Co(1)-O(2)	2.081(2)	Co(1)-N(1)	2.099(2)

Co(1)-O(1)	2.230(2)	O(2)-Co(1)-O(2)	154.73(12)
O(2)-Co(1)-N(1)	102.78(9)	N(1)-Co(1)-N(1)	92.78(13)
O(2)-Co(1)-O(1)	99.54(8)	N(1)-Co(1)-O(1)	93.61(9)
Compound **4**			
Zn(1)-O(1)	2.017(3)	Zn(1)-N(1)	2.097(3)
Zn(1)-O(2)	2.439(4)	O(1)-Zn(1)-O(1)	143.3(2)
O(1)-Zn(1)-N(1)	106.89(13)	N(1)-Zn(1)-N(1)	94.49(18)
N(1)-Zn(1)-O(2)	93.42(12)	O(2)-Zn(1)-O(2)	82.71(16)
Compound **5**			
Co(1)-O(2)	2.016(2)	Co(1)-O(3)	2.384(3)
Co(1)-O(4)	1.925(2)	Co(1)-N(2)	2.064(2)
Co(1)-N(3)	2.055(2)	O(4)-Co(1)-O(2)	98.10(11)
O(4)-Co(1)-N(3)	97.61(11)	O(2)-Co(1)-N(2)	103.86(10)
N(3)-Co(1)-N(2)	112.89(10)	O(4)-Co(1)-O(3)	151.17(10)
O(2)-Co(1)-O(3)	58.90(10)	N(3)-Co(1)-O(3)	85.23(10)
N(2)-Co(1)-O(3)	86.45(9)		
Compound **6**			
Cd(1)-O(3)	2.172(5)	Cd(1)-N(1)	2.271(4)
Cd(1)-N(2)	2.309(4)	Cd(1)-O(1)	2.357(4)
Cd(1)-O(2)	2.392(4)	O(3)-Cd(1)-N(1)	143.85(19)
O(3)-Cd(1)-N(2)	90.25(17)	N(1)-Cd(1)-N(2)	113.31(16)
O(3)-Cd(1)-O(1)	91.50(16)	N(1)-Cd(1)-O(1)	90.24(16)
N(2)-Cd(1)-O(1)	134.91(18)	O(3)-Cd(1)-O(2)	124.65(18)
N(1)-Cd(1)-O(2)	84.98(15)	N(2)-Cd(1)-O(2)	87.75(15)
O(1)-Cd(1)-O(2)	55.22(16)		

Powder X-ray diffraction patterns of compound 1-6

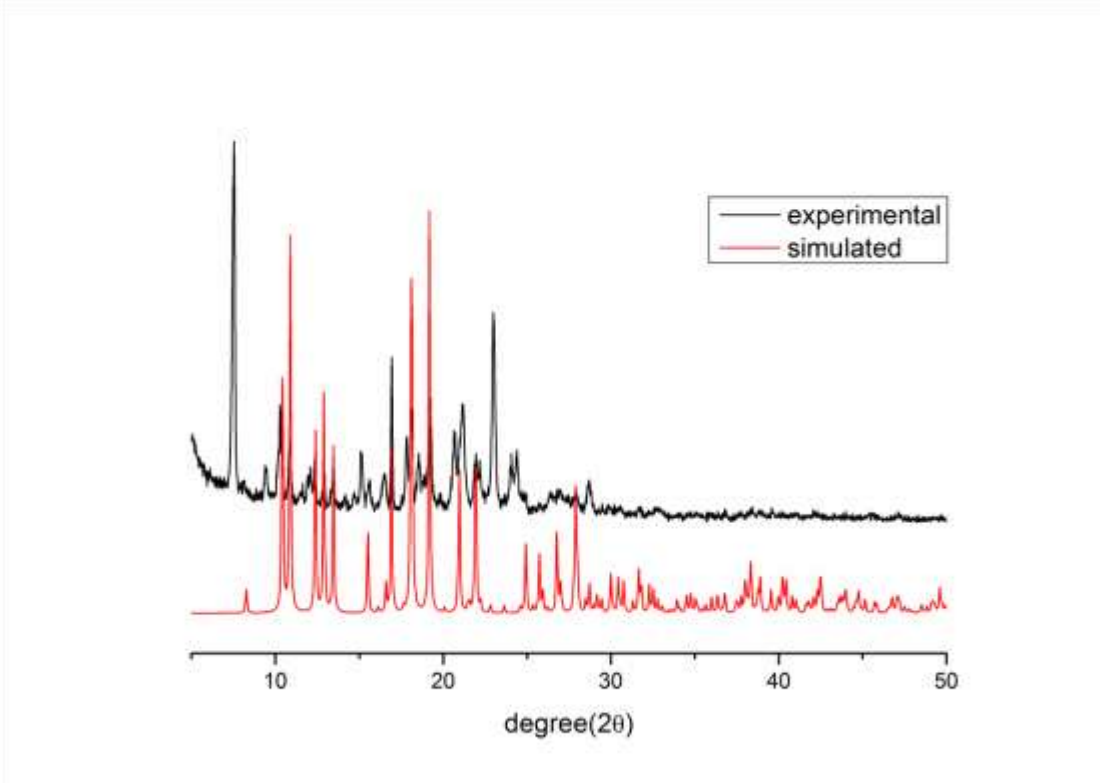

Fig. S1. Powder X-ray diffraction patterns of compound **1**

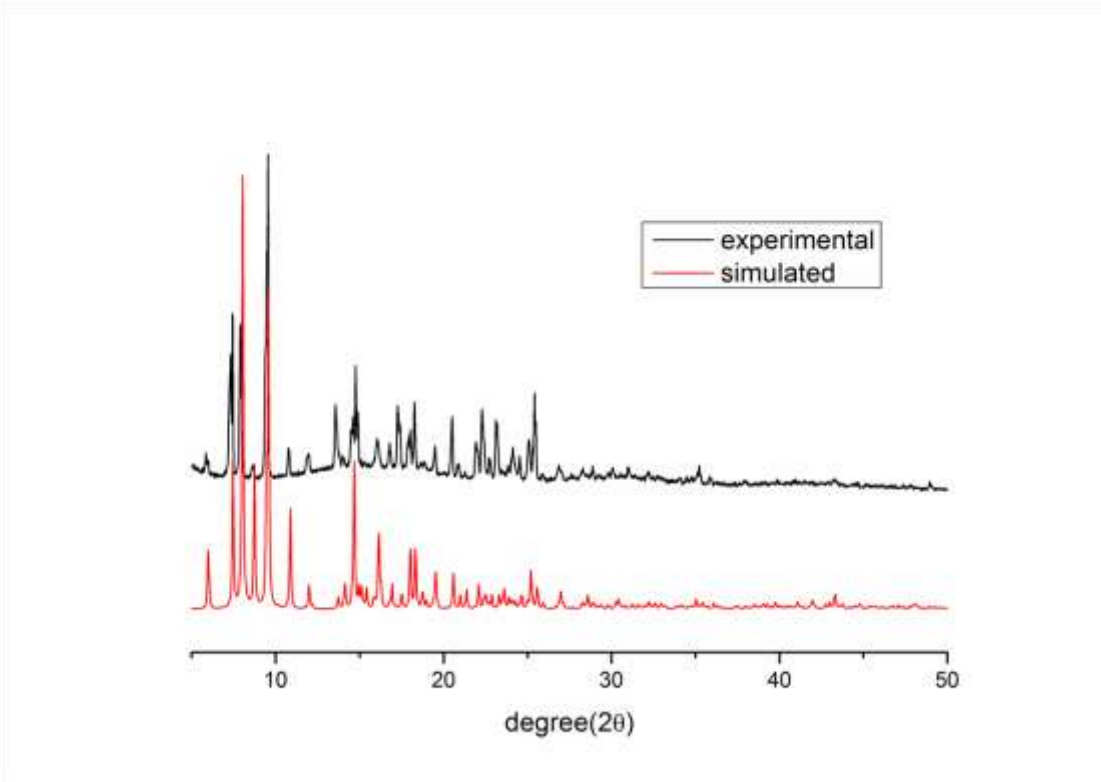

Fig. S2. Powder X-ray diffraction patterns of compound **2**

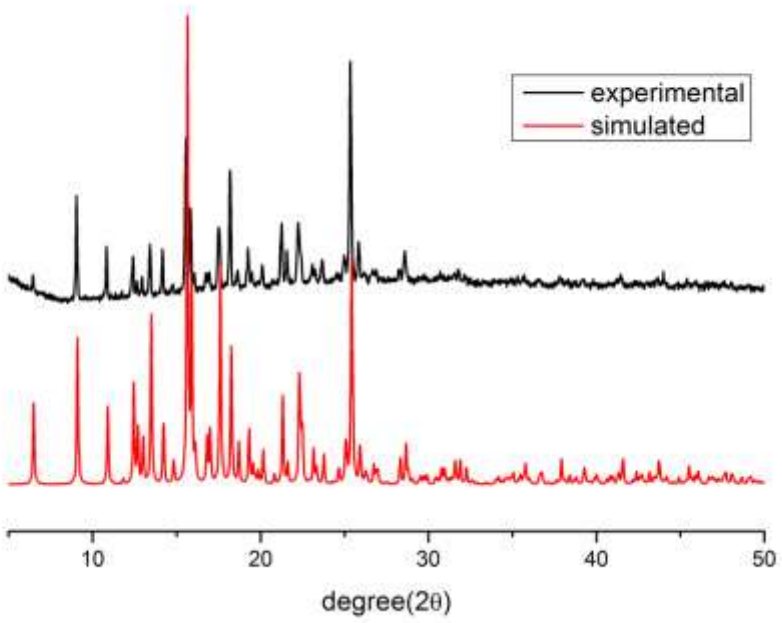

Fig. S3. Powder X-ray diffraction patterns of compound **3**

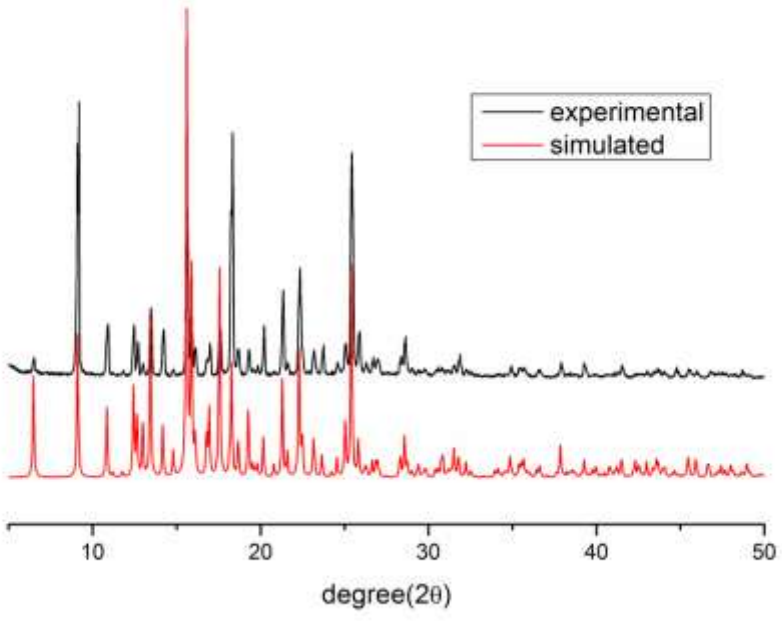

Fig. S4. Powder X-ray diffraction patterns of compound **4**

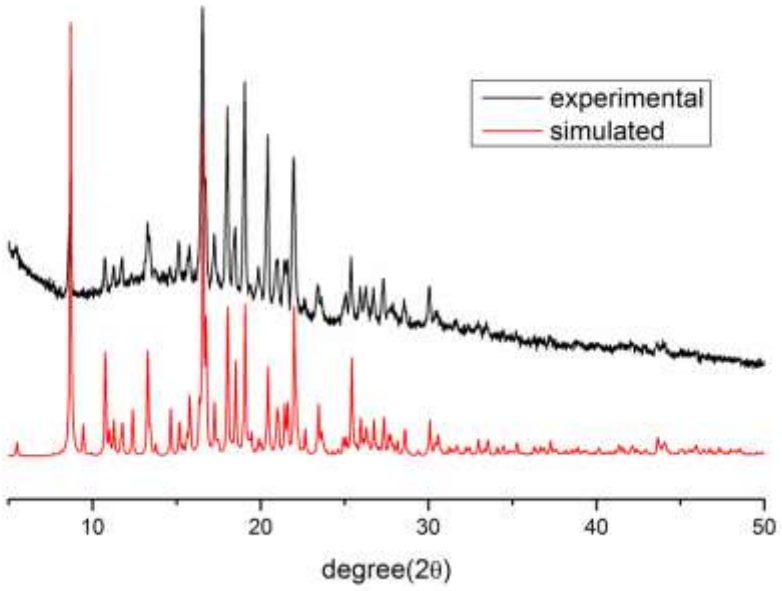

Fig. S5. Powder X-ray diffraction patterns of compound **5**

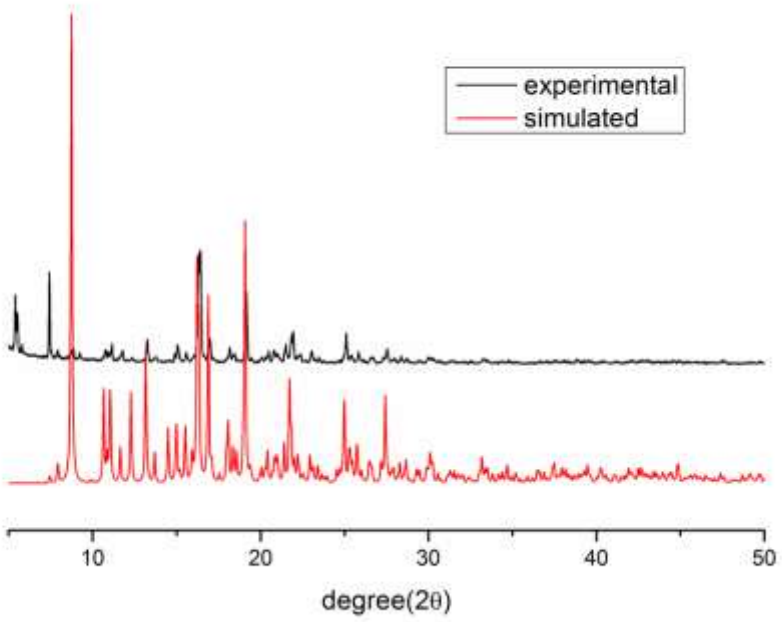

Fig. S6. Powder X-ray diffraction patterns of compound **6**

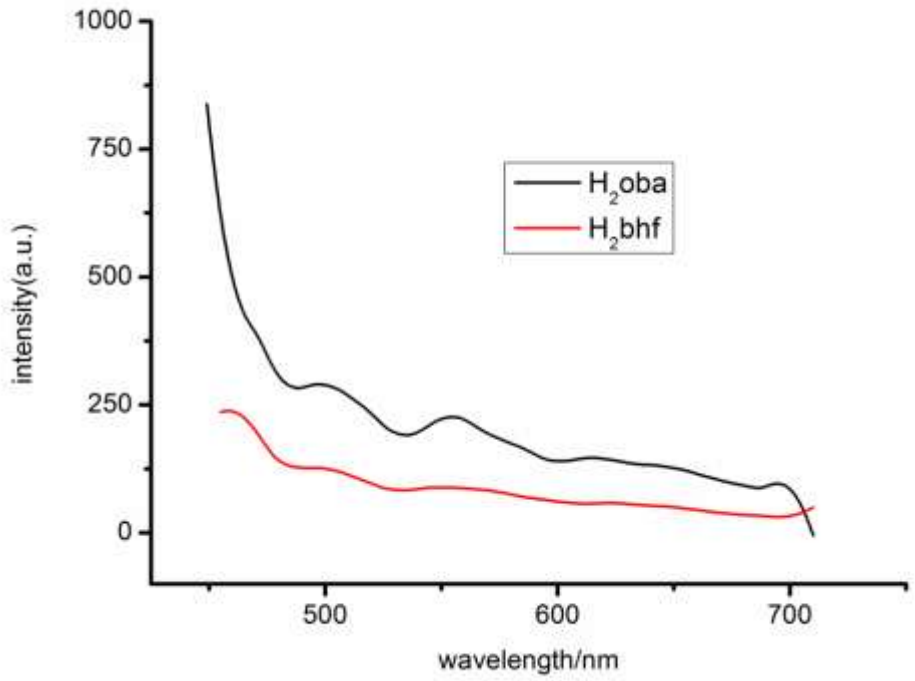

Fig. S7. Emission spectra of H_2oba and H_2bhf at room temperature.

Results of IR analysis in KBr pullet

Compound	IR (KBr)
1	3420(s), 1593(s), 1516(s), 1487(m), 1332(m), 1284(m), 1236(w), 1188(w), 995(w), 811(m), 753(m), 559(w), 512(w)
2	3423(s), 3037(w), 2920(w), 2360(s), 1597(s), 1490(m), 1394(m), 1336(w), 1288(m), 1220(w), 1182(w), 1055(w), 1017(w), 882(w), 824(m), 746(w)
3	3426(s), 3039(w), 1683(m), 1623(m), 1589(s), 1484(m), 1415(w), 1356(m), 1297(m), 1227(s), 1167(w), 928(w), 840(m), 802(s), 725(m), 560(m)
4	3414(s), 3085(w), 3046(w), 1934(w), 1597(s), 1558(m), 1481(s), 1403(m), 1326(m), 1288(s), 1259(w), 1210(w), 1166(m), 1065(w), 968(w), 930(w), 843(m), 805(s), 727(m), 563(m), 505(m)
5	3389(s), 3029(w), 1599(s), 1540(m), 1497(s), 1374(m), 1296(m), 1232(s), 1193(w), 833(m), 740(m), 575(w), 520(w)
6	3383(s), 3020(w), 1597(s), 1535(m), 1494(s), 1379(m), 1296(m), 1223(s), 1189(w), 1161(w), 1015(w), 891(w), 818(m), 746(m), 569(w), 517(w)

Table S2 Results of IR analysis of compounds **1** to **6** in KBr pullet