# Supporting Information

# Syntheses, structures, photoluminescence, and magnetic properties of four new metal-organic frameworks based on imidazole ligands and aromatic polycarboxylate acids

**Table S1 Selected Bond Distances (Å) and Angles (deg) for complexes**

| | | | |
|---|---|---|---|
| Complex **1** | | | |
| Cu1─O2 | 1.989(2) | Cu1─ N1 | 1.991(3) |
| Cu1─ O1_a | 1.999(3 | Cu1─ N5_b | 1.999(3) |
| Cu1─ O3 | 2.349(3) | Cu1─ O6_c | 2.394(3) |
| Cu2─ N10_b | 1.957(3) | Cu2─ N6 | 1.979(4) |
| Cu2─ O4 | 1.985(3) | Cu2─ O5 | 1.988(3) |
| | | | |
| O2─ Cu1─ N1 | 87.64(13) | O2─ Cu1─ O1_a | 179.29(11) |
| N1─ Cu1─ O1_a | 91.66(13) | O2─ Cu1─ N5_b | 89.69(13) |
| N1─ Cu1─ N5_b | 176.46(14) | O1_a─ Cu1─ N5_b | 91.02(13) |
| O2─ Cu1─ O3 | 91.10(11) | N1─ Cu1─ O3 | 90.19(13) |
| O1─ Cu1─ O3_a | 88.82(11) | N5─ Cu1─ O3_b | 92.19(13) |
| O2─ Cu1─ O6_c | 95.55(11) | N1─ Cu1─ O6_c | 89.66(12) |
| O1_a─ Cu1─ O6_c | 84.53(11) | N5_b─ Cu1─ O6_c | 88.27(12) |
| O3─ Cu1─O6_c | 173.34(10) | N10─Cu2─N6_b | 171.00(15) |
| N10─Cu2─O4 | 93.05(14) | N6─Cu2─O4 | 90.18(13) |
| N10─Cu2─O5_b | 87.80(14) | N6─Cu2─O5 | 90.15(14) |
| O4─Cu2─O5 | 172.13(12) | N10_b─Cu2─O4_d | 94.48(13) |
| N6─Cu2─O4_d | 94.41(12) | O4─Cu2─O4_d | 78.13(11) |
| O5─Cu2─O4_d | 94.00(11) | C3─N1─Cu1 | 124.8(3) |
| C1─N1─Cu1 | 128.9(3) | N11─O1─Cu1 | 124.3(2) |
| N11─O2─Cu1_c | 122.6(2) | N12─O3─Cu1 | 126.5(2) |
| N12─O4─Cu2 | 117.2(2) | Cu2─O4─Cu2_d | 101.87(11) |
| | | | |
| Complex **2** | | | |
| N1─Cd1 | 2.222(3) | Cd1─O2 | 2.205(2) |
| | | | |
| O2─ Cd1─ N1 | 111.88(9) | O2─Cd1─N1 | 111.88(9) |
| N1─Cd1─N1_a | 94.28(14) | C3─N1─Cd1 | 122.8(2) |
| C1─N1─Cd1 | 130.7(2) | C10─O2─Cd1 | 102.32(19) |
| O2─Cd1─O2_a | 88.78(11) | | |
| Complex **3** | | | |
| Co1─O1 | 2.078(3) | Co1─N3_a | 2.150(4) |

| | | | |
|---|---|---|---|
| Co1─N1 | 2.155(4) | Co2─N5 | 2.091(4) |
| Co2─O3 | 2.123(3) | Co2─O5 | 2.124(4) |
| | | | |
| O1─Co1─O1_b | 180.00 | O1─Co1─N3_a | 93.02(15) |
| N3_a─Co1─N3_c | 180.00(19) | O1─Co1─N1 | 92.62(15) |
| N3─Co1─N1_a | 96.85(17) | N1─Co1─N1_b | 180.0(19) |
| N5─Co2─N5_d | 180.000 | N5─Co2─O3 | 93.41(14) |
| O3─Co2─O3_d | 180.000(1) | O3─Co2─O5 | 93.41(14) |
| N5─Co2─O5_d | 90.44(16) | O5─Co2─O5 | 180.0 |
| C18─N1─Co1 | 122.3(4) | C19─N1─Co1 | 129.4(4) |
| C29─N3─Co1_e | 126.5(4) | C27─N3─Co1_e | 128.1(4) |
| C9─N5─Co2 | 122.7(4) | C11─N5─Co2 | 132.5(4) |
| C1─O1─Co1 | 138.5(4) | C8─O3─Co2 | 126.4(4) |
| | | | |
| Complex **4** | | | |
| Zn1─N1 | 1.991(2) | Zn1─N3 | 1.986(3) |
| Zn1─O3_a | 2.0080(2) | Zn1─O6 | 1.970(2) |
| | | | |
| O6- Zn1 -N3 | 109.03(12) | O6- Zn1- N1 | 110.33(12) |
| N3 -Zn1- N1 | 117.12(12) | O6- Zn1 -O3_b | 102.79(11) |
| N3- Zn1- O3_b | 105.02(12) | N1 -Zn1 -O3_b | 111.48(12) |
| C3- Zn1-N1 | 127.9(3) | C1-Zn1-N1 | 126.4(3) |
| C15- Zn1-O6 | 110.1(2) | C5- Zn1-N3 | 126.0(3) |
| C23 -Zn1-O3_a | 107.8(2) | | |

a = -*x* + 1, *y* -1/2 , -*z+3/2*; b= *x+1*, *y* , *z*; c= -*x+1*, *y* + 1/2 , -*z+3/2*; d= -*x* +*1*, -*y* + 1 , -*z+2* ( compond **1)**

a = *x*, -*y* + 3/2 , -*z* + 1/2. (compond **2**)

a = *x* + 1, *y* -*2* , *z*; b= -*x+1*, -*y* , -*z* + 1; c= -*x*, -*y* + 2 , *z+1*; d= -*x* +*1*, -*y* + 2 , -*z*; e = *x* - 1, *y*+ 2, *z*.( compond **3)**

a = *x* -1, *y* , *z*; b= *x*+1, *y* , *z*.( compond **4)**

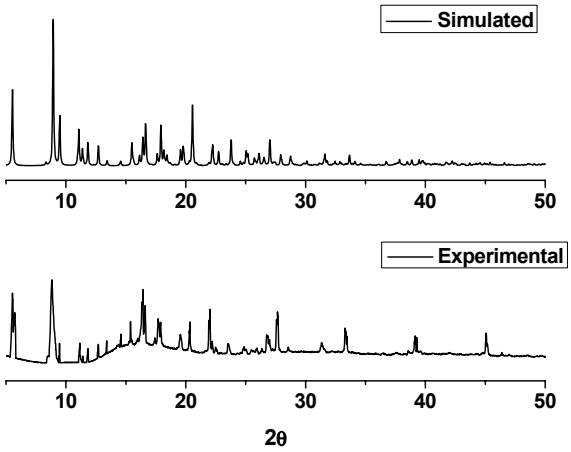


**Figure S1.** Experimental (bottom) and simulated (top) powder X-ray diffraction patterns of compound **1** at 293K.

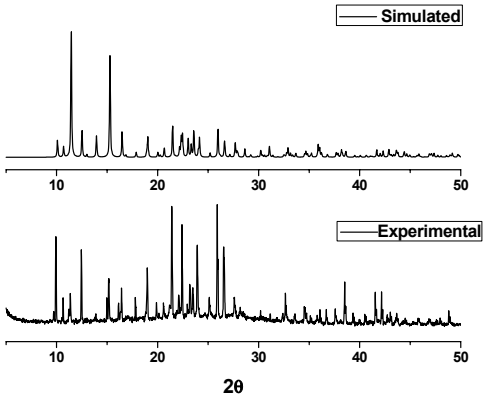


**Figure S2.** Experimental (bottom) and simulated (top) powder X-ray diffraction patterns of compound **2** at 293K.

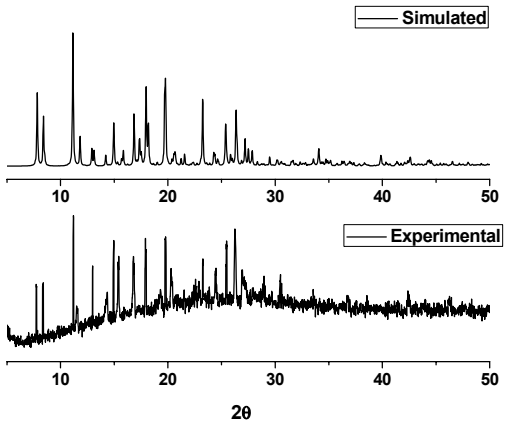


**Figure S3.** Experimental (bottom) and simulated (top) powder X-ray diffraction patterns of compound **3** at 293K.

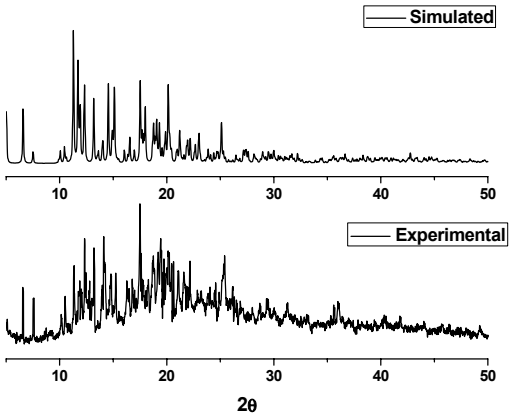


**Figure S4.** Experimental (bottom) and simulated (top) powder X-ray diffraction patterns of compound **4** at 293K.