Supporting Information for

Molecular Tectonics of Mixed-Ligand Metal-Organic Frameworks (MOFs): Positional Isomeric Effect, Metal-Directed Assembly and Structural Diversification

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Table S1. Pertinent Hydrogen-Bonding Parameters

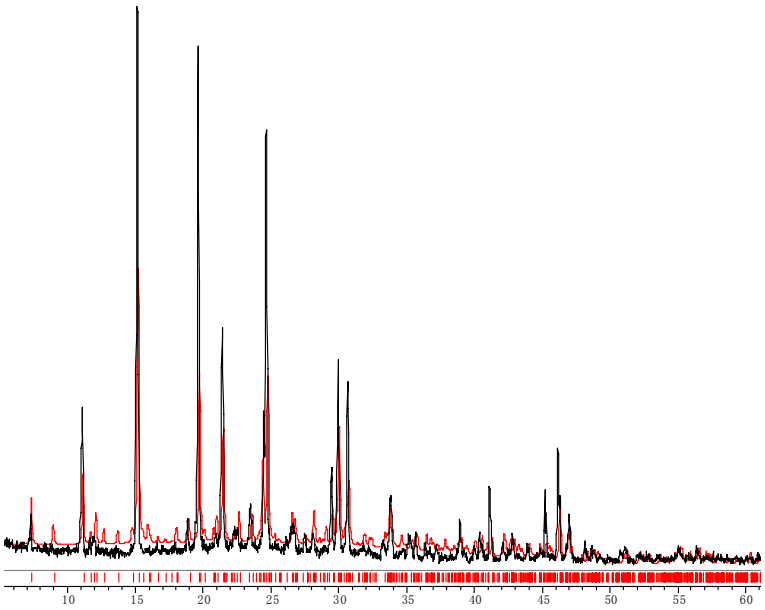
Complex	D–H···A	D···A (Å)	H···A (Å)	D–H···A (deg)
1	C4–H4···O1[a]	3.345(6)	2.57	141
	C10–H10···N5[b]	3.444(5)	2.56	159
4	O5–H5A···O9[c]	2.662(6)	1.85	160
	O9–H9A···O1[d]	2.819(6)	2.02	155
5	N5–H5A···O6	2.874(3)	2.07	149
	N11–H11A···O3[e]	2.898(3)	2.12	145
9	N5–H5A···O6[f]	2.921(5)	2.17	148
	O9–H9A···O1[g]	2.700(4)	1.85	177

[a] $x + 1/2, -y + 5/2, z - 1/2$. [b] $-x + 1, -y + 2, -z$. [c] $x + 1, y, z + 1$. [d] $-x + 1, -y + 2, -z + 1$. [e] $x - 1/2, -y + 1/2, z - 1/2$. [f] $-x + 1, -y, -z + 1$. [g] $-x + 2, -y - 1, -z$.

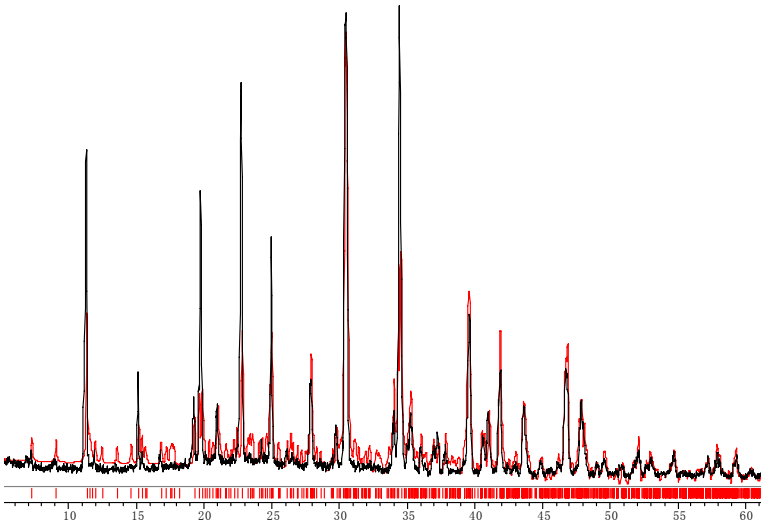
Table S2. Selective Bond Lengths (Å) and Angles (deg) for Complex **2**

Cd1–O1	2.269(3)	Cd1–O3A	2.280(3)
Cd1–O5	2.293(3)	Cd1–N6B	2.332(4)
Cd1–N1	2.339(4)	Cd1–O2A	2.354(3)
O1–C13	1.259(5)	O2–C13	1.238(5)
O3–C16	1.270(6)	O4–C16	1.231(6)
O1–Cd1–O3A	162.5(1)	O1–Cd1–O5	109.6(1)
O3A–Cd1–O5	86.7(1)	O1–Cd1–N6B	92.1(1)
O3A–Cd1–N6B	94.3(1)	O5–Cd1–N6B	90.3(1)
O1–Cd1–N1	81.7(1)	O3A–Cd1–N1	90.5(1)
O5–Cd1–N1	95.5(1)	N6B–Cd1–N1	172.7(1)
O1–Cd1–O2A	77.7(1)	O3A–Cd1–O2A	86.3(1)
O5–Cd1–O2A	172.7(1)	N6B–Cd1–N1	88.3(1)
N1–Cd1–O2A	86.6(1)		

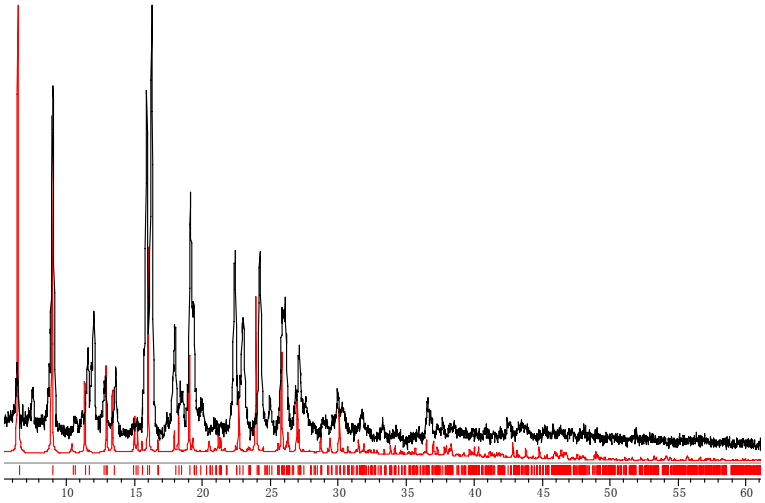
Symmetry codes: A $-x + 1/2, y + 1/2, -z + 1/2$; B $x - 1, y, z$.



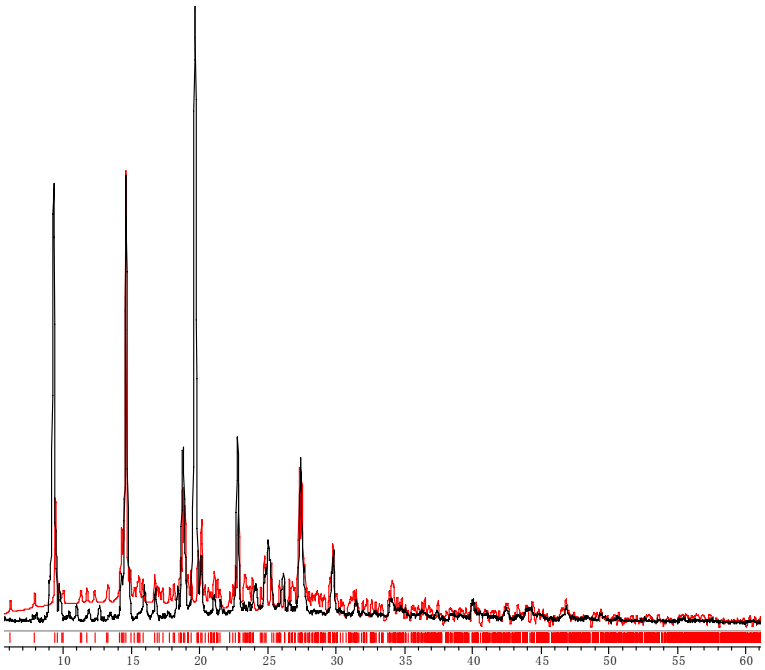
Complex 1



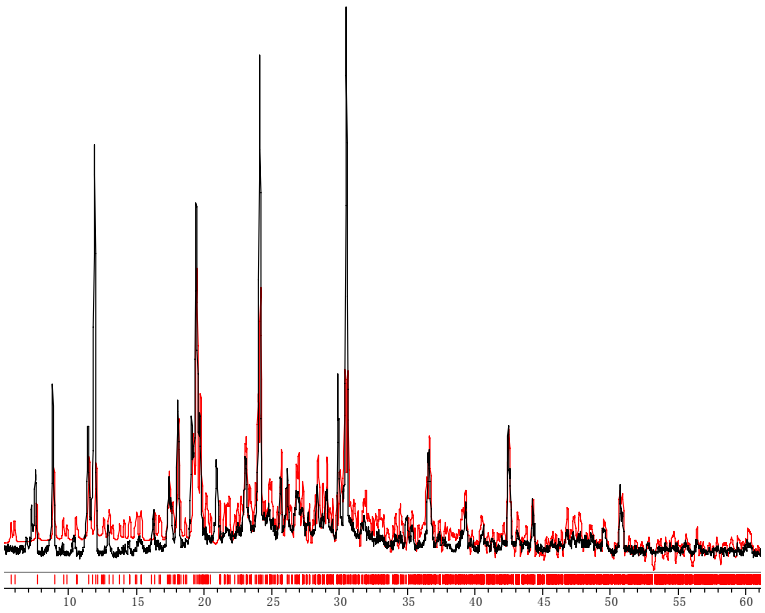
Complex 2



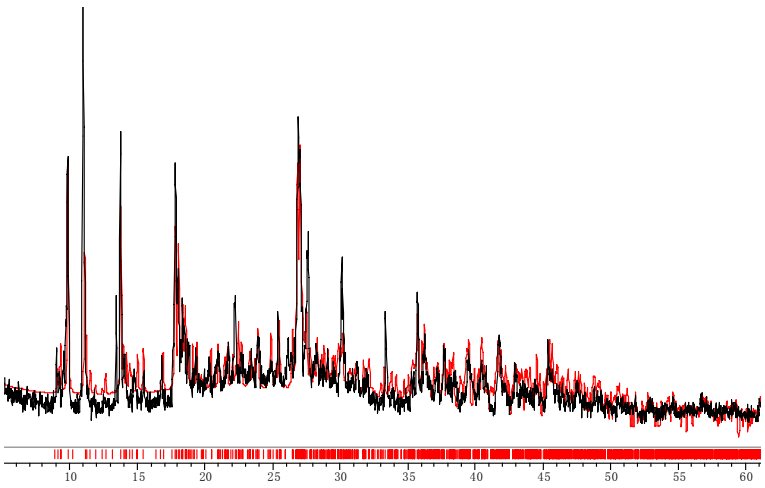
Complex 3



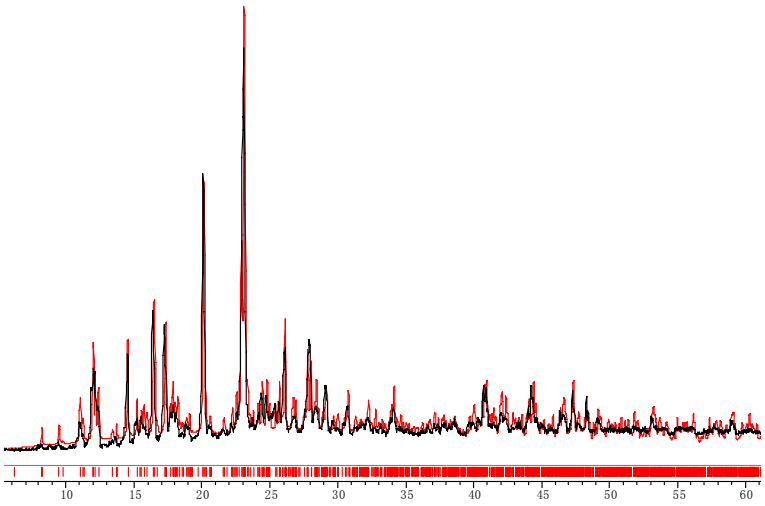
Complex 4



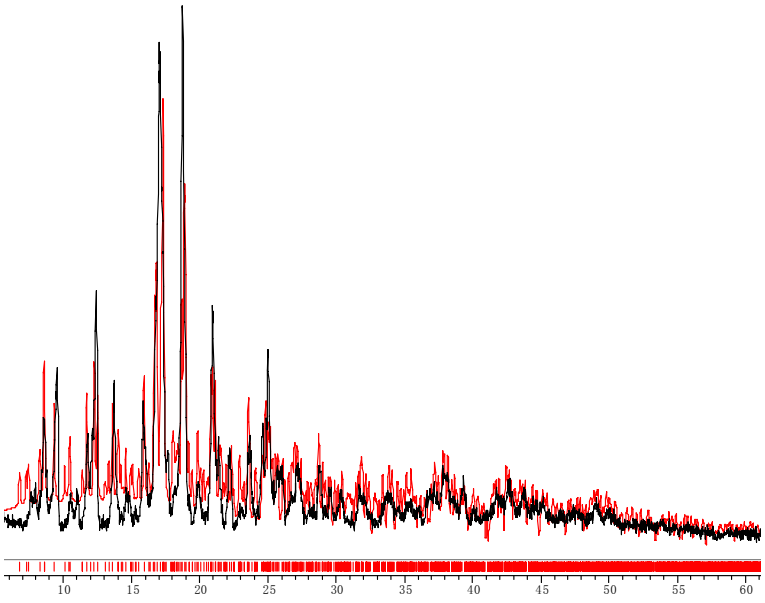
Complex 5



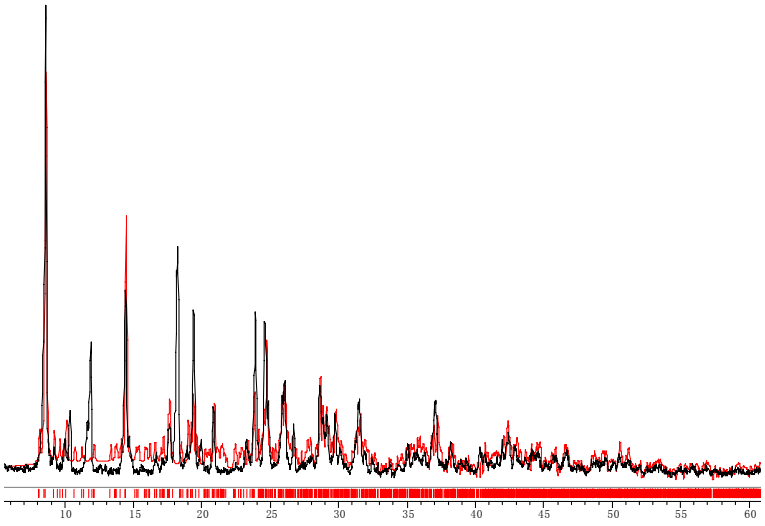
Complex 6



Complex 7



Complex 8



Complex 9

Figure S1. Experimental (black) and simulated (red) XRPD patterns for MOFs 1–9.

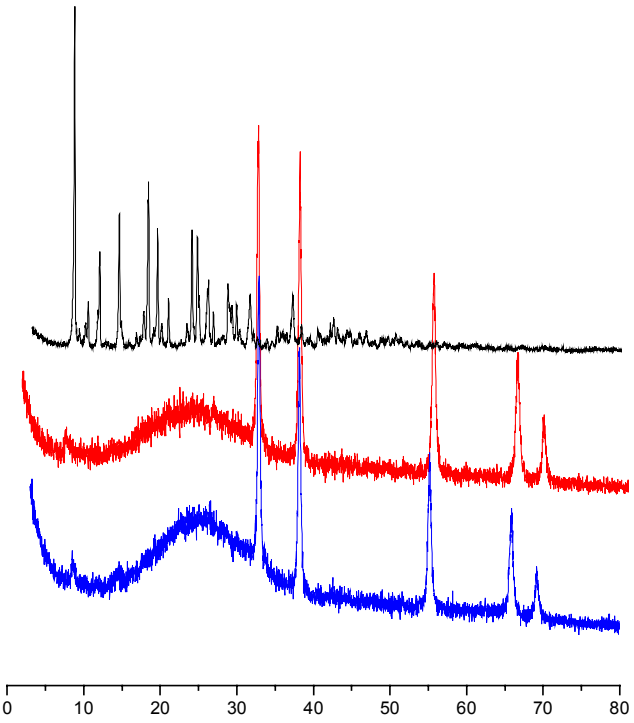
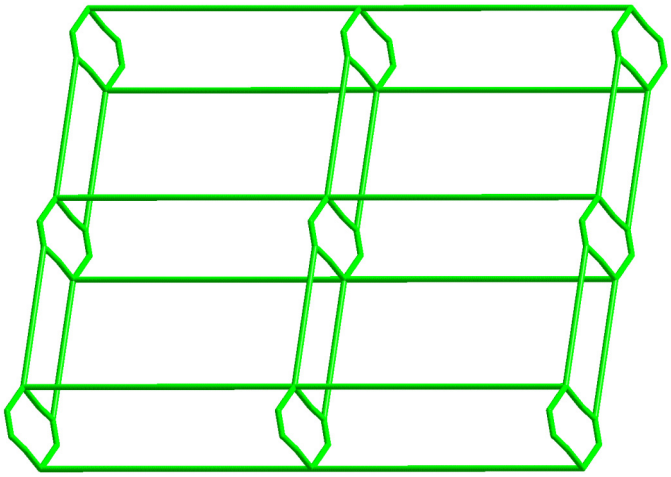
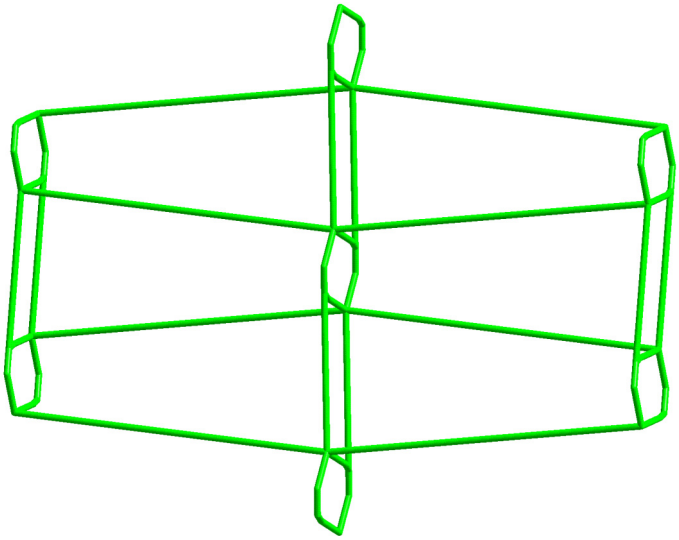


Figure S2. XRPD patterns for MOF 9 taken (black) at room temperature, (red) after removal of the guest solvents, and (blue) after reintroduction of the guest molecules.



(a)



(b)

Scheme 1. A schematic view showing the network connectivity of the dinuclear SBUs in MOFs 3 (a) and 5 (b).