Electronic Supplementary Material (ESI) for CrystEngComm

Structural diversity and properties of coordination polymers built from a semirigid tetradentenate carboxylic acid

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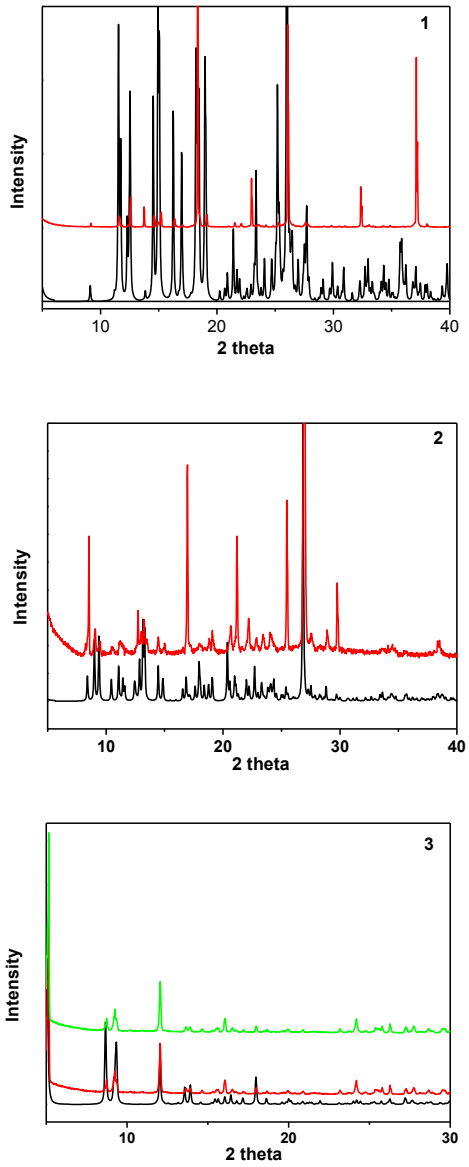

Figure S1. PXRD patterns for **1**-**3**: the as-synthesized (red), the simulated based on X-ray single-crystal data (black) and the activated sample (green).

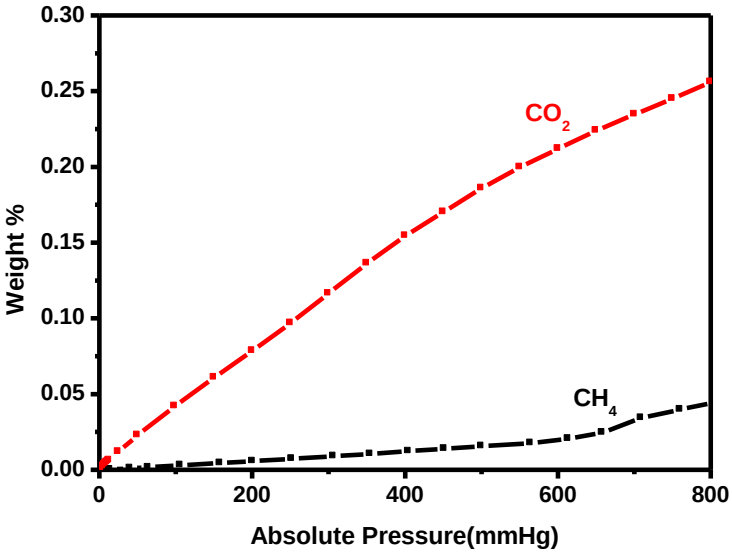

Figure S2. CH_4 and CO_2 adsorption isotherms for **3** at 273 K.

Table S1. Selected bond distances (Å) and angles (deg) for **1**–**3**

1			
Zn1–O1	2.168(3)	Zn1–O2	1.964(3)
Zn1–O3	2.117(3)	Zn1–O4^{iii}	1.940(3)
Zn1–O5	1.951(3)		
O2–Zn1–O1	92.47(13)	O2–Zn1–O3	86.90(12)
O3–Zn1–O1	172.84(13)	O4^{iii}–Zn1–O1	88.75(12)
O4^{iii}–Zn1–O2	135.10(11)	O4^{iii}–Zn1–O3	86.68(12)
O4^{iii}–Zn1–O5	129.96(12)	O5–Zn1–O1	91.50(12)
O5–Zn1–O2	94.89(12)	O5–Zn1–O3	95.66(13)
2			
Co1–O9	2.040(2)	Co1–O10	2.414(2)
Co1–O11	2.014(3)	Co1–O1W	2.096(3)
Co1–O1W^{ii}	2.302(3)	Co1–O2W	2.458(6)
O9–Co1–O1W	135.02(10)	O9–Co1–O1W^{ii}	87.26(10)
O11–Co1–O9	90.47(11)	O11–Co1–O1W	129.06(10)
O11–Co1–O1W^{ii}	87.77(10)	O1W–Co1–O1W^{ii}	75.55(11)
3			
Cd1–O1	2.243(4)	Cd1–O7^{v}	2.315(3)
Cd1–O10^{iii}	2.285(4)	Cd2–O2^{vii}	2.186(4)
Cd2–O3^{viii}	2.301(4)	Cd2–O4^{viii}	2.381(4)
Cd2–O7	2.326(3)	Cd2–O8	2.493(4)
Cd2–O9^{ix}	2.310(4)	Cd2–O10^{ix}	2.645(4)
O1–Cd1–O1^{ii}	179.999(1)	O1–Cd1–O7^{v}	90.08(13)
O1–Cd1–O7^{vi}	89.92(13)	O1–Cd1–O10^{iii}	91.26(14)
O1–Cd1–O10^{iv}	88.74(14)	O10^{iii}–Cd1–O10^{iv}	180.000(1)
O10^{iii}–Cd1–O7^{v}	77.22(14)	O10^{iv}–Cd1–O7^{v}	102.78(14)

$O2^{vii}$–Cd2–$O3^{viii}$	154.23(14)	$O2^{vii}$–Cd2–$O4^{viii}$	98.22(13)
$O2^{vii}$–Cd2–O7	100.22(14)	$O2^{vii}$–Cd2–O8	88.31(14)
$O2^{vii}$–Cd2–$O9^{ix}$	95.53(14)	$O2^{vii}$–Cd2–$O10^{ix}$	99.11(14)
$O3^{viii}$–Cd2–$O4^{viii}$	56.06(13)	$O3^{viii}$–Cd2–O7	98.59(13)
$O3^{viii}$–Cd2–O8	88.88(13)	$O3^{viii}$–Cd2–$O9^{ix}$	89.31(13)
$O3^{viii}$–Cd2–$O10^{ix}$	103.76(13)	$O4^{viii}$–Cd2–O8	87.57(12)
$O4^{viii}$–Cd2–$O10^{ix}$	144.60(13)	O7–Cd2–$O4^{viii}$	135.78(12)
O7–Cd2–O8	53.43(12)	O7–Cd2–$O10^{ix}$	70.20(13)
O8–Cd2–$O10^{ix}$	123.51(12)	$O9^{ix}$–Cd2–$O4^{viii}$	95.68(13)
$O9^{ix}$–Cd2–O7	121.86(13)	$O9^{ix}$–Cd2–O8	174.56(13)
$O9^{ix}$–Cd2–$O10^{ix}$	52.10(13)		

Symmetry transformations used to generate equivalent atoms: For **1**: i, -x+1, -y+1, -z; iii, -x+1, -y+1, -z+1. For **2**: ii, -x+2, -y+2, -z+2. For **3**: i, x, y-1, z-1; ii, -x+1, -y+1, -z-1; iii, x-1, y, z-1; iv, -x+2, -y+1, -z; v, x, y, z-1; vi, -x+1, -y+1, -z; vii, x, y, z+1; viii, x, y+1, z+1; ix, x-1, y, z.

Table S2. Hydrogen-Bonding Geometries (Å, deg) for **1** and **2**

D–H…A	dD…A	dH…A	∠D–H…A
1			
O3–H3A…O8	2.691	1.79	154
O9–H9C…O4	2.679	1.76	160
O12–H12D…O8	3.087	2.21	151
2			
O1W–H1X…O3	2.722	1.93	155
O1W–H1Y…O2	2.708	1.88	165
O2W–H2Y…O9	3.248	2.57	137
O4–H4C…O8	3.213	2.55	126
O8–H8A…O13	2.614	1.69	160
O14–H14C…O7	2.598	1.84	134
C3–H3…O4W	3.279	2.36	170
C22–H22…O1	3.450	2.6	152
C33–H33A…O6	3.532	2.59	163