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Supporting Materials

Tuning cadmium coordination architectures by 1,4-bis(1,2,4-triazol-1-ylmethyl)benzene and sulfoisophthalate

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Table S1 Selected bond lengths [Å] and angles [°] for **1**, **2** and **3**.

		1	
Cd(1)-N(3)	2.287(6)	Cd(1)-O(8)	2.322(7)
Cd(1)-O(9)	2.290(6)	Cd(2)-O(1)	2.298(5)
Cd(2)-O(2)	2.555(4)	Cd(2)-O(3)#2	2.532(4)
Cd(2)-O(4)#2	2.403(5)	Cd(2)-N(6)	2.325(6)
Cd(2)-N(9)	2.294(6)	Cd(2)-N(12)	2.341(6)
N(3)-Cd(1)-N(3)#1	180.000(1)	O(9)#1-Cd(1)-O(9)	180.00(7)
O(8)#1-Cd(1)-O(8)	180.000(3)	N(3)-Cd(1)-O(8)	84.7(2)
N(3)-Cd(1)-O(9)	87.0(2)	O(9)-Cd(1)-O(8)	91.4(3)
O(1)-Cd(2)-O(2)	52.81(17)	O(1)-Cd(2)-O(3)#2	133.06(17)
O(1)-Cd(2)-O(4)#2	81.00(17)	O(3)#2-Cd(2)-O(2)	173.58(16)
O(4)#2-Cd(2)-O(2)	133.37(16)	O(4)#2-Cd(2)-O(3)#2	52.89(16)
O(1)-Cd(2)-N(6)	89.6(2)	N(9)-Cd(2)-O(1)	144.01(18)
O(1)-Cd(2)-N(12)	84.2(2)	N(6)-Cd(2)-O(2)	92.26(18)
N(9)-Cd(2)-O(2)	91.36(17)	N(12)-Cd(2)-O(2)	83.89(18)
N(6)-Cd(2)-O(3)#2	85.48(18)	N(9)-Cd(2)-O(3)#2	82.91(18)
N(12)-Cd(2)-O(3)#2	98.84(18)	N(6)-Cd(2)-O(4)#2	93.60(19)
N(9)-Cd(2)-O(4)#2	133.82(18)	N(12)-Cd(2)-O(4)#2	85.66(18)
N(9)-Cd(2)-N(6)	95.7(2)	N(6)-Cd(2)-N(12)	173.9(2)
N(9)-Cd(2)-N(12)	89.2(2)		
		2	
Cd(1)-O(1)	2.621(3)	Cd(1)-O(2)	2.320(3)
Cd(1)-O(4)#1	2.293(2)	Cd(1)-O(8)	2.345(3)
Cd(1)-N(3)	2.289(3)	Cd(1)-N(9)	2.327(3)

Cd(2)-O(9)	2.330(3)	Cd(2)-O(10)	2.309(4)
Cd(2)-N(6)	2.264(4)		
O(2)-Cd(1)-O(1)	52.56(9)	O(4)#1-Cd(1)-O(1)	137.53(8)
O(8)-Cd(1)-O(1)	80.54(10)	O(4)#1-Cd(1)-O(2)	88.40(9)
O(2)-Cd(1)-O(8)	93.07(10)	O(4)#1-Cd(1)-O(8)	86.43(10)
N(3)-Cd(1)-O(1)	78.59(9)	N(3)-Cd(1)-O(2)	127.53(10)
N(3)-Cd(1)-O(4)#1	143.41(9)	N(3)-Cd(1)-O(8)	96.91(10)
N(9)-Cd(1)-O(1)	107.13(11)	O(2)-Cd(1)-N(9)	90.63(10)
O(4)#1-Cd(1)-N(9)	86.82(11)	N(9)-Cd(1)-O(8)	172.20(11)
N(3)-Cd(1)-N(9)	86.22(11)	O(9)#2-Cd(2)-O(9)	180.000(1)
O(10)-Cd(2)-O(10)#2	180.000(1)	N(6)-Cd(2)-N(6)#2	180.000(1)
O(10)-Cd(2)-O(9)	97.63(13)	N(6)-Cd(2)-O(9)	90.07(13)
N(6)-Cd(2)-O(10)	86.14(14)		

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Cd(1)-O(1)	2.285(3)	Cd(1)-O(2)	2.650(4)
Cd(1)-O(10)#1	2.459(4)	Cd(1)-O(11)#1	2.414(4)
Cd(1)-O(15)	2.265(4)	Cd(1)-O(16)	2.312(4)
Cd(1)-N(3)	2.280(4)	Cd(2)-O(3)	2.438(4)
Cd(2)-O(4)	2.367(4)	Cd(2)-O(8)	2.261(4)
Cd(2)-O(17)	2.372(4)	Cd(2)-O(18)	2.271(4)
Cd(2)-N(9)	2.263(4)	Cd(3)-O(19)	2.350(5)
Cd(3)-O(20)	2.246(5)	Cd(3)-O(21)	2.280(5)
Cd(3)-O(22)	2.299(5)	Cd(3)-N(6)	2.313(5)
Cd(3)-N(12)#2	2.265(7)		
O(1)-Cd(1)-O(2)	51.90(12)	O(1)-Cd(1)-O(10)#1	135.95(13)
O(1)-Cd(1)-O(11)#1	82.62(12)	O(15)-Cd(1)-O(1)	87.95(14)
O(1)-Cd(1)-O(16)	89.37(13)	O(10)#1-Cd(1)-O(2)	171.75(12)
O(11)#1-Cd(1)-O(2)	134.03(11)	O(15)-Cd(1)-O(2)	93.91(14)
O(16)-Cd(1)-O(2)	83.50(14)	O(11)#1-Cd(1)-O(10)#1	53.44(12)
O(15)-Cd(1)-O(10)#1	89.27(14)	O(16)-Cd(1)-O(10)#1	93.48(14)
O(15)-Cd(1)-O(11)#1	90.29(14)	O(16)-Cd(1)-O(11)#1	90.52(14)
O(15)-Cd(1)-O(16)	177.07(13)	N(3)-Cd(1)-O(1)	139.89(14)
N(3)-Cd(1)-O(2)	88.00(14)	N(3)-Cd(1)-O(10)#1	84.06(14)
N(3)-Cd(1)-O(11)#1	136.87(13)	O(15)-Cd(1)-N(3)	96.84(15)
N(3)-Cd(1)-O(16)	84.47(14)	O(4)-Cd(2)-O(3)	54.05(12)
O(8)-Cd(2)-O(3)	138.99(13)	O(17)-Cd(2)-O(3)	96.61(14)
O(18)-Cd(2)-O(3)	87.23(15)	O(8)-Cd(2)-O(4)	85.89(13)
O(4)-Cd(2)-O(17)	88.61(15)	O(18)-Cd(2)-O(4)	96.30(16)
O(8)-Cd(2)-O(17)	90.07(15)	O(8)-Cd(2)-O(18)	89.14(15)
O(18)-Cd(2)-O(17)	174.96(16)	N(9)-Cd(2)-O(3)	88.61(14)
N(9)-Cd(2)-O(4)	141.44(15)	O(8)-Cd(2)-N(9)	132.28(15)
N(9)-Cd(2)-O(17)	86.40(16)	N(9)-Cd(2)-O(18)	90.45(16)
O(20)-Cd(3)-O(19)	91.9(2)	O(21)-Cd(3)-O(19)	174.7(2)
O(22)-Cd(3)-O(19)	83.3(2)	O(20)-Cd(3)-O(21)	89.1(2)

O(20)-Cd(3)-O(22)	87.6(2)	O(21)-Cd(3)-O(22)	91.6(2)
N(6)-Cd(3)-O(19)	91.63(19)	O(20)-Cd(3)-N(6)	172.9(2)
O(21)-Cd(3)-N(6)	86.87(19)	O(22)-Cd(3)-N(6)	86.7(2)
N(12)#2-Cd(3)-O(19)	84.5(3)	O(20)-Cd(3)-N(12)#2	94.4(2)
N(12)#2-Cd(3)-O(21)	100.6(3)	N(12)#2-Cd(3)-O(22)	167.7(3)
N(12)#2-Cd(3)-N(6)	92.1(2)		

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

Table S2 Hydrogen bonds for **1**, **2** and **3** (Å and °).

D-H···A	d(D-H)	d(H···A)	D(D···A)	<(DHA)
		1		
O(8)-H(1W)···O(12)^{i}	0.86(2)	1.88(3)	2.731(13)	174(15)
O(8)-H(2W)···O(14)	0.87(2)	1.90(6)	2.708(12)	155(13)
O(9)-H(3W)···O(5)^{ii}	0.84(2)	1.89(4)	2.714(8)	166(15)
O(9)-H(5W)···O(10)^{iii}	0.83(2)	1.97(2)	2.737(10)	152(5)
O(10)-H(5W)···O(4)^{iv}	0.89(2)	2.24(8)	2.883(9)	129(8)
O(10)-H(6W)···O(12)^{v}	0.89(2)	2.50(2)	2.945(14)	111(2)
		2		
O(8)-H(1W)···O(4)^{i}	0.888(19)	2.03(3)	2.800(4)	145(3)
O(8)-H(2W)···O(2)^{ii}	0.876(19)	1.90(2)	2.749(4)	164(4)
O(9)-H(3W)···O(11)^{iii}	0.889(18)	1.84(2)	2.713(5)	166(3)
O(9)-H(4W)···O(7)^{iv}	0.860(18)	2.52(3)	3.317(7)	155(3)
O(10)-H(5W)···O(7)^{iv}	0.859(19)	1.84(2)	2.643(5)	155(4)
O(10)-H(6W)···O(12)^{v}	0.873(19)	1.88(2)	2.752(5)	173(4)
O(11)-H(7W)···O(3)	0.916(18)	1.85(2)	2.742(4)	165(4)
O(11)-H(8W)···O(5)^{i}	0.910(19)	1.86(2)	2.759(5)	170(4)
O(12)-H(9W)···O(1)	0.907(18)	2.10(2)	2.998(5)	169(4)
O(12)-H(10W)···O(5)^{i}	0.911(19)	2.22(3)	3.026(6)	148(3)
		3		
O(15)-H(1W)···O(3)^{a}	0.869(19)	1.918(19)	2.662(5)	143(2)
O(15)-H(2W)···O(24)	0.871(19)	2.03(2)	2.715(6)	135(3)
O(16)-H(3W)···O(8)^{b}	0.892(19)	1.92(4)	2.692(6)	144(5)
O(16)-H(4W)···O(4)^{b}	0.876(19)	2.05(4)	2.723(5)	133(5)
O(17)-H(5W)···O(11)^{c}	0.876(19)	2.26(3)	2.811(5)	121(3)
O(17)-H(6W)···N(9)	0.881(19)	2.52(2)	3.174(6)	131.1(17)
O(18)-H(7W)···O(10)^{d}	0.891(19)	2.14(3)	2.767(5)	127(3)
O(18)-H(8W)···O(23)^{a}	0.892(19)	1.84(2)	2.728(6)	172(6)
O(19)-H(9W)···N(12)^{e}	0.896(19)	2.49(4)	3.104(12)	126(3)
O(19)-H(10W)···N(5)^{f}	0.90(2)	2.57(5)	3.11(3)	119(4)
O(20)-H(11W)···O(26)^{g}	0.89(2)	1.99(3)	2.765(12)	145(5)
O(20)-H(12W)···O(24)^{h}	0.891(19)	1.98(2)	2.865(8)	171(7)
O(21)-H(13W)···O(25)^{g}	0.88(2)	1.88(2)	2.757(9)	170(7)

O(21)-H(14W)···O(27)^{i}	0.88(2)	2.03(4)	2.861(10)	157(7)
O(22)-H(15W)···N(2)^{j}	0.91(2)	1.97(3)	2.841(7)	162(6)
O(22)-H(16W)···O(6)^{h}	0.89(2)	1.92(3)	2.780(6)	162(7)
O(23)-H(17W)···O(13)^{b}	0.89(2)	2.46(3)	3.211(12)	142(4)
O(23)-H(17W)···O(12)^{b}	0.89(2)	2.56(4)	3.373(13)	152(5)
O(23)-H(18W)···O(9)^{i}	0.88(2)	1.92(3)	2.756(7)	158(6)
O(24)-H(19W)···O(7)^{k}	0.886(19)	1.96(2)	2.814(6)	161(4)
O(24)-H(20W)···O(2)^{a}	0.893(19)	1.87(3)	2.709(6)	155(5)

Symmetry transformations used to generate equivalent atoms:i -x+2, -y+3, -z+1; ii -x+2, -y+2, -z+1; iii x+1, y+1, z; iv -x, -y+1, -z+1; v -x+1, -y+2, -z+1 for **1**; i -x+2, -y+1, -z+2; ii -x+1, -y+1, -z+2; iii -x+3, -y+1, -z+1; iv x+1, y, z-1; v x+1, y, z for **2**; a -x+2, -y+1, -z+2; b -x+1, -y+1, -z+2; c -x, -y+1, -z+1; d -x+1, -y+1, -z+1; e x+2, y, z+1; f -x+4, -y, -z+2; g x+1, y-1, z+1; h x+1, y-1, z; i x+1, y, z+1; j -x+3, -y, -z+2; k x+1, y, z for **3**.

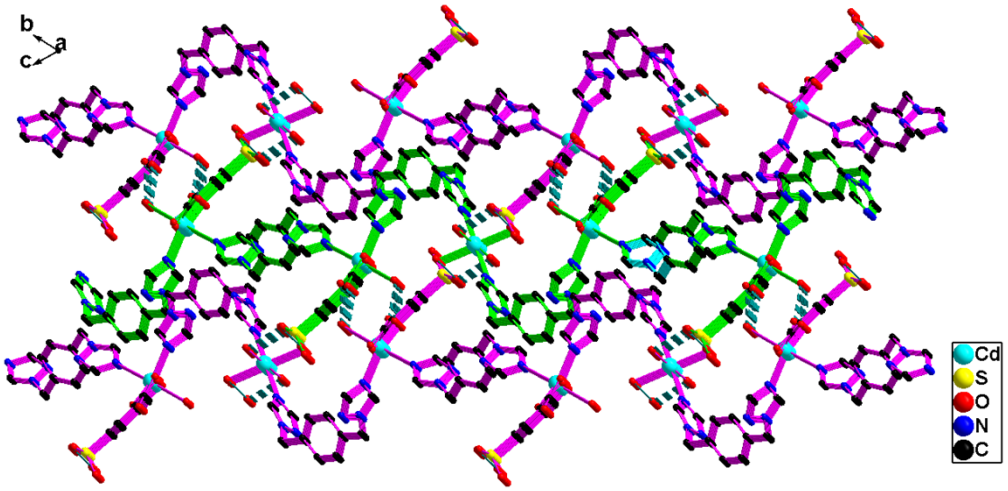

Fig. S1 A 3D hydrogen bond network in **2**.

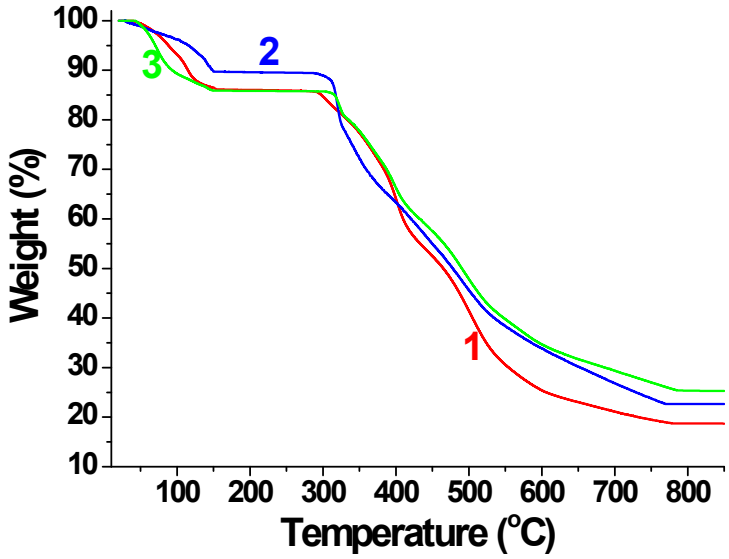

Fig. S2 The TG curves of **1**, **2** and **3**.