Supplementary Material (ESI) for CrystEngComm

Supplementary information

Title: Self-assembled coordination polymers of V-shaped bis(pyridyl)thiadiazole dependent upon the spacer length and flexibility of aliphatic dicarboxylate ligands

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Table S1. Selected bond angles (°) of complexes 1–6 [a]

1				**2**			
O3–Cu1–O1	174.6(2)	O3–Cu1–O4#2	77.0 (2)	O1–Cu2–O5	93.25(9)	O4–Cu1–O2	88.52(9)
O3–Cu1–O2#1	91.0(2)	O1–Cu1–O4#2	100.5(2)	O4–Cu1–N2	92.6 (1)	O1–Cu2–N1#3	91.4 (1)
O1–Cu1–O2#1	83.9(2)	O2#1–Cu1–O4#2	85.7(2)	N1#3–Cu2–O5	85.3 (1)	N2–Cu1–O2	90.1(1)
O3–Cu1–N2	95.3(2)	N2–Cu1–O4#2	103.3(2)				
O1–Cu1–N2	90.0(2)	O3–Cu1–O4#3	92.1(2)				
O2#1–Cu1–N2	169.9(2)	O1–Cu1–O4#3	89.8(2)				
O2#1–Cu1–O4#3	88.2(2)	O4#2-Cu1–O4#3	167.5(2)				
N2–Cu1–O4#3	83.7(2)						
3				**4**			
O1–Cu1–N1	100.4(3)	O2#2–Cu1–O1	168.5(3)	O1–Cu1–O3	176.5 (2)	O1–Cu1–N2#1	86.9 (2)
O4#1–Cu1–O2#2	90.1(3)	O3#3–Cu1–O1	90.6(3)	O1–Cu1–N1	89.6 (2)	O3–Cu1–N2#1	91.5(2)
O4#1–Cu1–O3#3	168.8(3)	O3#3–Cu1–N1	100.7(3)	O3–Cu1–N1	91.8(2)	N1–Cu1–N2#1	175.3 (2)
O2#2–Cu1–O3#3	87.3(3)	O2#2–Cu1–N1	91.1(3)				
O4#1–Cu1–O1	89.7(3)						
5				**6**			
O1–Cu1–O3#1	146.6(2)	N1–Cu1–N4#2	169.0(2)	O4#1–Cd1–O1	89.4(3)	O3–Cd1–O5	92.0(4)
O1–Cu1–N1	92.8(2)	O1–Cu1–O2#3	125.0(2)	O4#1–Cd1–O3	170.2(3)	O2#2–Cd1–O5	93.4(4)
O3#1–Cu1–N1	88.3 (2)	O3#1–Cu1–O2#3	88.4 (2)	O1–Cd1–O3	81.4 (2)	O4#1–Cd1–N1	83.6(2)
O1–Cu1–N4#2	92.7(2)	N1–Cu1–O2#3	84.6(2)	O4#1–Cd1–O2#2	100.0 (2)	O1–Cd1–N1	84.0(3)
O3#1–Cu1–N4#2	92.4 (2)	N4#2–Cu1–O2#3	84.4(2)	O1–Cd1–O2#2	170.1(3)	O3–Cd1–N1	91.9(2)
				O3–Cd1–O2#2	88.9(3)	O2#2–Cd1–N1	94.3(2)
				O4#1–Cd1–O5	91.4(4)	O5–Cd1–N1	171.5(4)
				O1–Cd1–O5	89.1(4)		

[a] Symmetry codes: **1**: #1 -x+1/2, -y+3/2, -z; #2 -x+1/2, -y+1/2, -z; #3 -x+1/2,y+1/2,-z+1/2. **2**: #3 x, y+1, z+1. **3**: #1 x, -y+1/2, z-1/2; #2 -x+2, -y+1, -z+1; #3 -x+2, y+1/2, -z+3/2. **4**: #1 x, y-1, z-1. **5**: #1 x-1/2, y, -z+1; #2 x, y+1, z; #3 -x+1, y, -z+1/2. **6**: #1 -x+3/2, y-1/2, z-1/2; #2 -x+3/2, y-1/2, z+1/2.

Table S2. Selected bond angles (°) of complexes 7–10 [a]

7				**8**			
O4#1–Cd1–O2	165.00(5)	O2–Cd1–N1	87.95(5)	N1–Cd1–N4#1	170.1(2)	N4#1–Cd1–O2	90.3(2)
O4#1–Cd1–O4#2	71.62(6)	O4#2–Cd1–N1	93.81(6)	N1–Cd1–O1	91.6(2)	O1–Cd1–O2	53.8(2)
O2–Cd1–O4#2	93.50(5)	O1–Cd1–N1	94.53(5)	N4#1–Cd1–O1	93.4(2)	O4#2–Cd1–O2	88.4(2)
O4#1–Cd1–O1	139.10(5)	N2#3–Cd1–N1	179.08(5)	N1–Cd1–O4#2	84.5(2)	O3#3–Cd1–O2	144.6(2)
O2–Cd1–O1	55.86(5)	O4#1–Cd1–O3#1	52.32(5)	N4#1–Cd1–O4#2	86.3(2)	N1–Cd1–O4#3	87.6(2)
O4#2–Cd1–O1	147.82(5)	O2–Cd1–O3#1	142.48(5)	O1–Cd1–O4#2	142.2(2)	N4#1–Cd1–O4#3	93.5(2)
O4#1–Cd1–N2#3	88.95(5)	O4#2–Cd1–O3#1	123.93(5)	N1–Cd1–O3#3	94.3(2)	O1–Cd1–O4#3	142.9(2)
O2–Cd1–N2#3	91.77(5)	O1–Cd1–O3#1	87.51(5)	N4#1–Cd1–O3#3	94.1(3)	O4#2–Cd1–O4#3	74.6(2)
O4#2–Cd1–N2#3	85.33(5)	N2#3–Cd1–O3#1	93.60(5)	O1–Cd1–O3#3	90.9(2)	O3#3–Cd1–O4#3	52.3(2)
O1–Cd1–N2#3	86.03(5)	N1–Cd1–O3#1	87.16(5)	O4#2–Cd1–O3#3	126.9(2)	O2–Cd1–O4#3	162.3(2)
O4#1–Cd1–N1	91.09(5)			N1–Cd1–O2	85.8(2)		
9				**10**			
O7–Cd1–O1	113.5(2)	N1–Cd2–N4#4	172.2(2)	N1–Cd1–O3	85.7(2)	O3–Cd1–O1	152.5(2)
O7–Cd1–O4#1	148.3(2)	O7–Cd1–N3#2	82.3(3)	N1–Cd1–O2	128.5(2)	O2–Cd1–O1	54.0(2)
O1–Cd1–O4#1	89.7(2)	O1–Cd1–N3#2	80.9(3)	O3–Cd1–O2	145.8(2)	O5–Cd1–O1	79.4(2)
O7–Cd1–N2	97.2(2)	O4#1–Cd1–N3#2	80.0(6)	N1–Cd1–O5	102.8(2)	O4#1–Cd1–O1	103.0(2)
O1–Cd1–N2	93.0(2)	N2–Cd1–N3#2	173.0(2)	O3–Cd1–O5	82.1(2)	N1–Cd1–O4	131.6(2)
O4#1–Cd1–N2	103.1(2)	O5–Cd1–N3#2	96.9(3)	O2–Cd1–O5	88.8(2)	O3–Cd1–O4	53.9(2)
O7–Cd1–O5	79.5(2)	O4–Cd2–N4#4	98.7(2)	N1–Cd1–O4#1	87.0(2)	O2–Cd1–O4	95.1(2)
O1–Cd1–O5	166.2(2)	O2–Cd2–N1	102.2(2)	O3–Cd1–O4#1	98.7 (2)	O5–Cd1–O4	97.2(2)
O4#1–Cd1–O5	76.5(2)	O2–Cd2–O5#3	146.0(2)	O2–Cd1–O4#1	85.2(2)	O4#1–Cd1–O4	75.8(2)
N2–Cd1–O5	89.9(2)	N1–Cd2–O5#3	98.3(2)	O5–Cd1–O4#1	170.3(2)	O1–Cd1–O4	148.8(2)
O5#3–Cd2–N4#4	79.7(2)	O2–Cd2–O8	119.1(2)	N1–Cd1–O1	78.8(2)		
O8–Cd2–N4#4	81.3(3)	N1–Cd2–O8	92.1(2)				
O8–Cd2–O4	162.6(2)	O5#3–Cd2–O8	86.7(2)				
O2–Cd2–N4#4	83.2(2)	O2–Cd2–O4	77.8(2)				
O5#3–Cd2–O4	76.1(2)	N1–Cd2–O4	88.0(2)				

[a] Symmetry codes: **7**: #1 -x+1, y-1/2, -z+1/2; #2 x, -y+3/2, z-1/2; #3 x+1, y+1, z. **8**: #1 x, y-1, z-1; #2 -x+1, -y, -z; #3 x-1, y, z. **9**: #1 x, y-1, z; #2 x-1/2, -y+1/2, z; #3 x, y+1, z; #4 x+1/2, -y+3/2, z. **10**: #1 -x+1, -y, -z+1.

Table S3. Possible hydrogen bond geometries for complexes 1, 2 and 5 [a]

Complex	D–H···A (Å)	D–H (Å)	H···A (Å)	D···A (Å)	<DHA (°)
1	O11–H11A···O2#6	0.80	1.98	2.774(7)	173
	O11–H11B···O13#7	0.80	2.00	2.899(4)	147
	O12–H12B···O2#6	0.80	2.11	2.905(6)	173
	O13–H13B···O11#8	0.80	2.27	2.839(5)	129
2	O7–H7WA···N4#6	0.83	2.16	2.951(4)	159
	O7–H7WB···O6	0.83	1.99	2.796(4)	164
	O6–H6WB···O3#7	0.83	2.06	2.873(4)	168
	O6–H6WA···O3#8	0.83	2.02	2.855(4)	175
	O5–H5WB···O7	0.82	2.26	3.077(4)	176
	O5–H5WA···O2	0.83	2.09	2.742(3)	136
5	O6–H6B···O4#8	0.80	2.01	2.810(6)	178
	O6–H6A···N3#7	0.80	2.23	3.031(6)	179
	O5–H5WB···O6#6	0.83	2.06	2.773(8)	144
	O5–H5WA···O6	0.84	1.92	2.711(9)	156

[a] Symmetry codes: **1**: #6 x, -y+2, z+1/2; #7 x, y+1, z; #8 x, -y+1, z-1/2. **2**: #6 x, y+1, z; #7 -x+1, -y+1, -z+1; #8 x, y, z-1. **5**: #6 -x+3/2, -y+1, z; #7 -x+1, -y+1, -z+1; #8. -x+3/2, y-1, z+1/2

Table S4. A comparison of the structural features for complexes 1–10

Complex	Metal ion	Coordination number	Anion	C···C[a] / Å	Coordination net	Interpenetration
1	Cu	6	ox	1.524	3D	none
2	Cu	6	mal	2.566	2D→H-bonding 3D	2-fold
3	Cu	5	glu	4.352	2D	none
4	Cu	5+2	adi	5.420	3D	2-fold
5	Cu	5	fum	3.884	3D	2-fold
6	Cd	6	mal	2.531	2D	none
7	Cd	7	suc	3.184	3D	polyknotting
8	Cd	7	glu	4.153	2D double layers	none
9	Cd	6+1	male	3.124	2D	none
10	Cd	7	fum	3.874	2D	none

[a] The distance between two terminal backbone C-donors of aliphatic dicarboxylates.

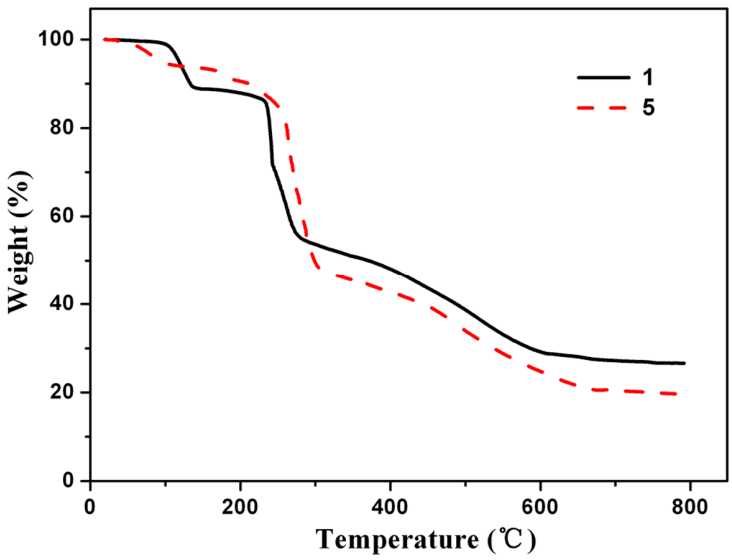
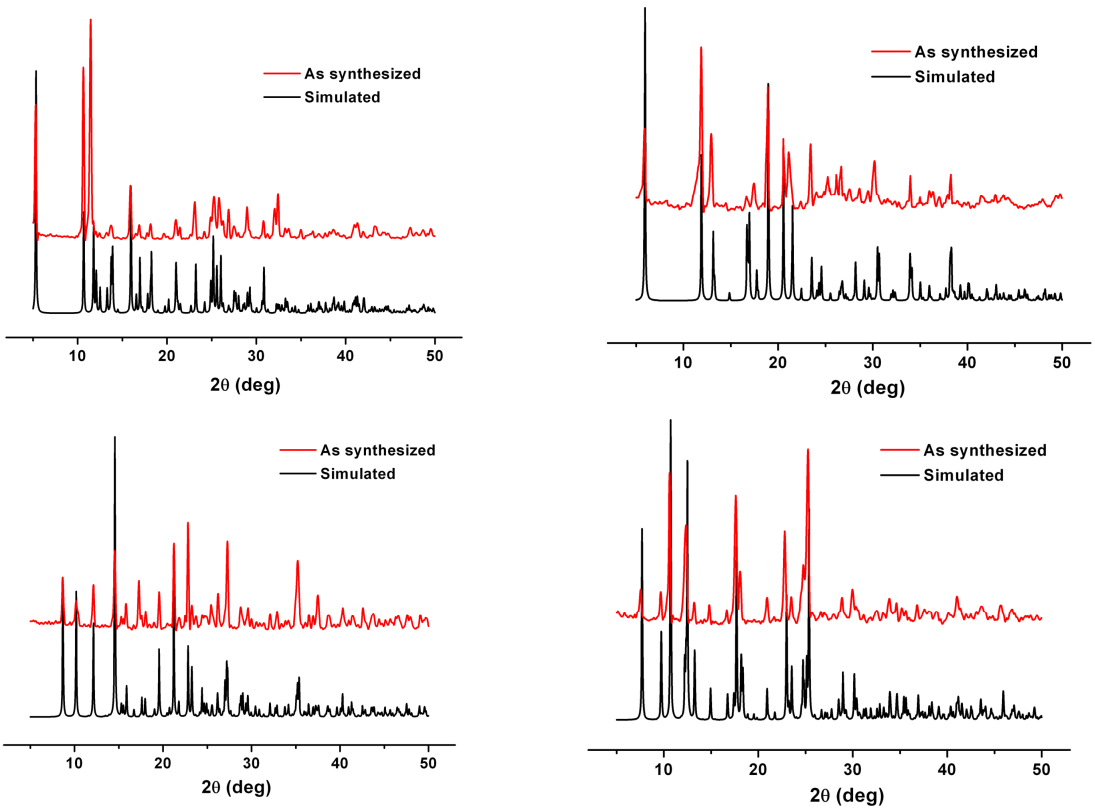


Fig. S1. TG graphs of complexes **1** (solid line) and **5**(dash line).



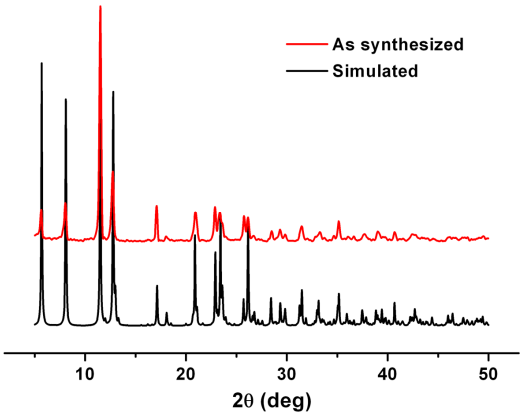


Fig. S2. Comparison of XRPD patterns of the simulated pattern from the single-crystal structure determination and the as-synthesized phases in complex **6** (a), complex **7** (b), complex **8** (c), complex **9** (d), and complex **10** (e).