Electronic Supplementary Information (ESI)

Topological Modulation of Metal-thiadiazole Dicarboxylate Coordination Polymers through Auxiliary Ligand Alteration

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Table S1. Selected bond lengths (Å) and angles (°) for **1**[a]

Co1—O2	2.052(2)	Co1—O3	2.086(2)
Co1—O4$^{\#1}$	2.0860(19)	Co1—N2	2.172(2)
Co1—O1W	2.087(2)	Co1—N1	2.178(2)
O2—Co1—O4$^{\#1}$	172.52(8)	O1W—Co1—N2	87.90(9)
O2—Co1—O1W	84.21(8)	O3—Co1—N2	90.94(9)
O4$^{\#1}$—Co1—O1W	100.69(8)	O2—Co1—N1	88.39(9)
O2—Co1—O3	89.93(8)	O4^{i}—Co1—N1	85.85(9)
O4$^{\#1}$—Co1—O3	85.33(7)	O1W—Co1—N1	91.47(9)
O1W—Co1—O3	173.84(8)	O3—Co1—N1	90.27(9)
O2—Co1—N2	97.06(9)	N2—Co1—N1	174.42(9)
O4$^{\#1}$—Co1—N2	88.81(9)		

[a]Symmetry code: #1: $-x+1/2, y-1/2, -z+1/2$.

Table S2. Selected bond lengths (Å) and angles (°) for **2**[a]

Co1—O4	2.098(2)	Co1—N3	2.136(3)
Co1—N4	2.114(3)	Co1—O5	2.149(3)
Co1—O1	2.120(2)	Co1—N2	2.197(3)
O4—Co1—N4	88.51(9)	O1—Co1—O5	88.13(11)
O4—Co1—O1	172.67(9)	N3—Co1—O5	173.77(13)
N4—Co1—O1	90.19(9)	O4—Co1—N2	104.59(9)
O4—Co1—N3	91.28(10)	N4—Co1—N2	166.56(9)
N4—Co1—N3	89.92(10)	O1—Co1—N2	76.43(9)
O1—Co1—N3	95.93(10)	N3—Co1—N2	92.72(10)
O4—Co1—O5	84.79(11)	O5—Co1—N2	83.62(10)
N4—Co1—O5	94.80(11)		

Table S3. Selected bond lengths (Å) and angles (°) for **3**[a]

Zn1—O3$^{\#1}$	2.002(8)	Zn1—N3	2.105(10)
Zn1—O1W	2.031(9)	Zn1—O2$^{\#1}$	2.181(8)
Zn1—O1	2.054(8)	Zn1—N1	2.408(10)
O3$^{\#1}$—Zn1—O1W	86.5(3)	O1—Zn1—O2$^{\#1}$	86.6(4)
O3$^{\#1}$—Zn1—O1	168.1(3)	N3—Zn1—O2$^{\#1}$	87.3(4)
O1W—Zn1—O1	98.0(4)	O3$^{\#1}$—Zn1—N1	96.2(3)
O3$^{\#1}$—Zn1—N3	97.1(4)	O1W—Zn1—N1	92.5(4)
O1W—Zn1—N3	98.9(4)	O1—Zn1—N1	72.7(3)
O1—Zn1—N3	93.1(4)	N3—Zn1—N1	163.0(4)
O3$^{\#1}$—Zn1—O2$^{\#1}$	87.7(3)	O2$^{\#1}$—Zn1—N1	82.6(3)
O1W—Zn1—O2$^{\#1}$	172.0(4)		

[a]Symmetry code: #1: x, $-y+1$, $z+1/2$.

Table S4. Selected bond lengths (Å) and angles (°) for **4**[a]

Zn1—O2	2.004(6)	Zn1—O6	2.045(6)
Zn1—O1W	2.032(6)	Zn1—O3	2.093(6)
Zn1—O4$^{\#1}$	2.038(5)	Zn1—N2$^{\#1}$	2.534(7)
O2—Zn1—O1W	86.2(2)	O4$^{\#1}$—Zn1—O3	88.9(2)
O2—Zn1—O4$^{\#1}$	167.0(2)	O6—Zn1—O3	84.3(2)
O1W—Zn1—O4$^{\#1}$	94.6(2)	O2—Zn1—N2$^{\#1}$	96.0(2)
O2—Zn1—O6	101.6(3)	O1W—Zn1—N2$^{\#1}$	93.6(3)
O1W—Zn1—O6	100.5(3)	O4$^{\#1}$—Zn1—N2$^{\#1}$	71.0(2)
O4$^{\#1}$—Zn1—O6	90.9(3)	O6—Zn1—N2$^{\#1}$	158.0(2)
O2—Zn1—O3	89.2(2)	O3—Zn1—N2$^{\#1}$	82.8(2)
O1W—Zn1—O3	174.0(3)		

[a]Symmetry code: #1: x, $-y+1/2$, $z-1/2$.

Table S5. Selected bond lengths (Å) and angles (°) for **5**[a]

Zn1—O3	1.970(3)	Zn1—N3	2.036(3)
Zn1—O1$^{\#2}$	2.009(3)	Zn1—N8$^{\#3}$	2.039(3)
O3—Zn1—O1$^{\#2}$	105.44(13)	O3—Zn1—N8$^{\#3}$	104.99(14)
O3—Zn1—N3	120.58(14)	O1$^{\#2}$—Zn1—N8$^{\#3}$	124.86(14)
O1$^{\#2}$—Zn1—N3	97.10(14)	N3—Zn1—N8$^{\#3}$	105.27(14)

[a]Symmetry codes: #2: $-x$, $-y+2$, $-z+1$; #3: $-x+3/2$, $y+1/2$, z.

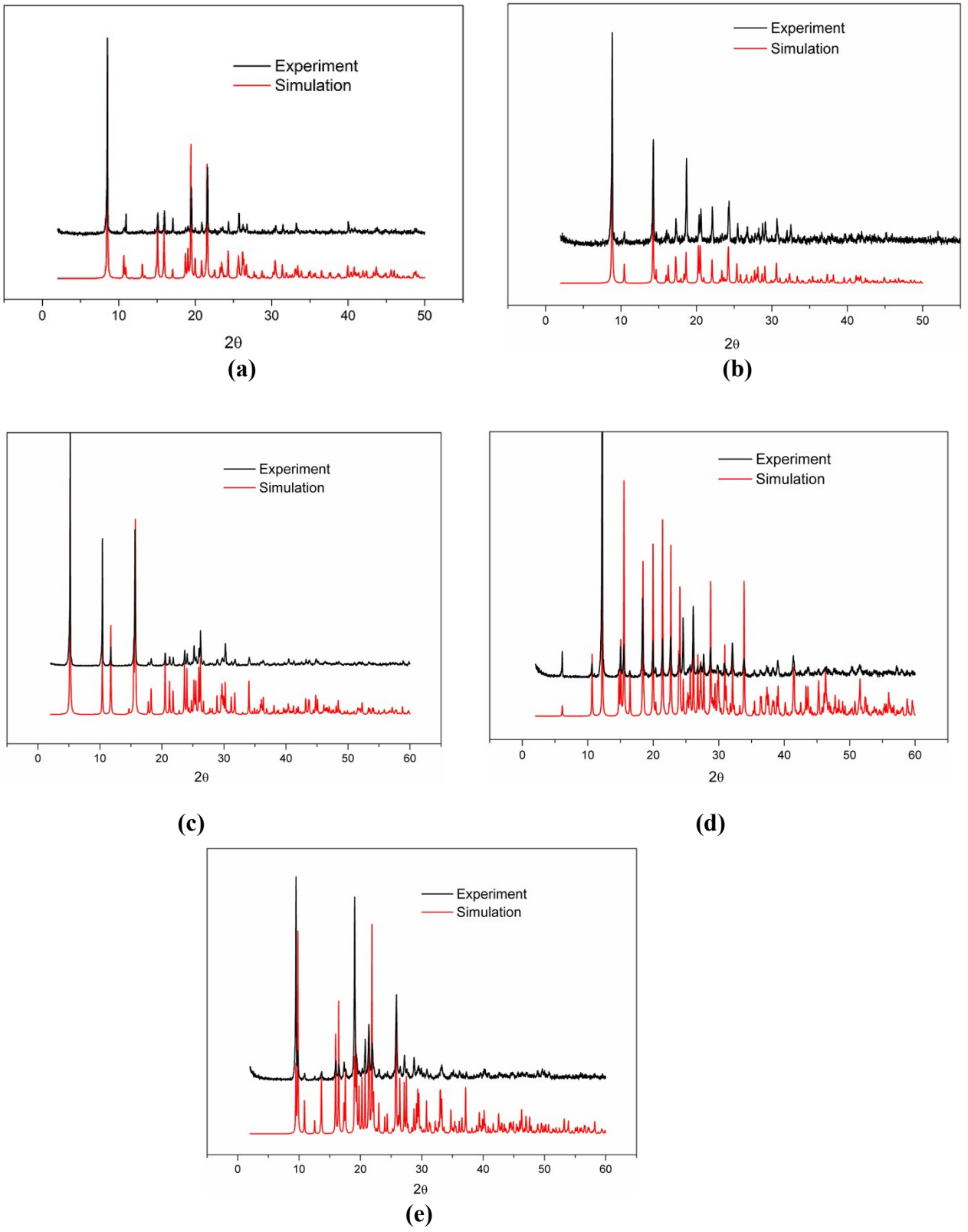

Figure S1. PXRD patterns of (a) **1**, (b) **2**, (c) **3**, (d) **4** and (e) **5**.

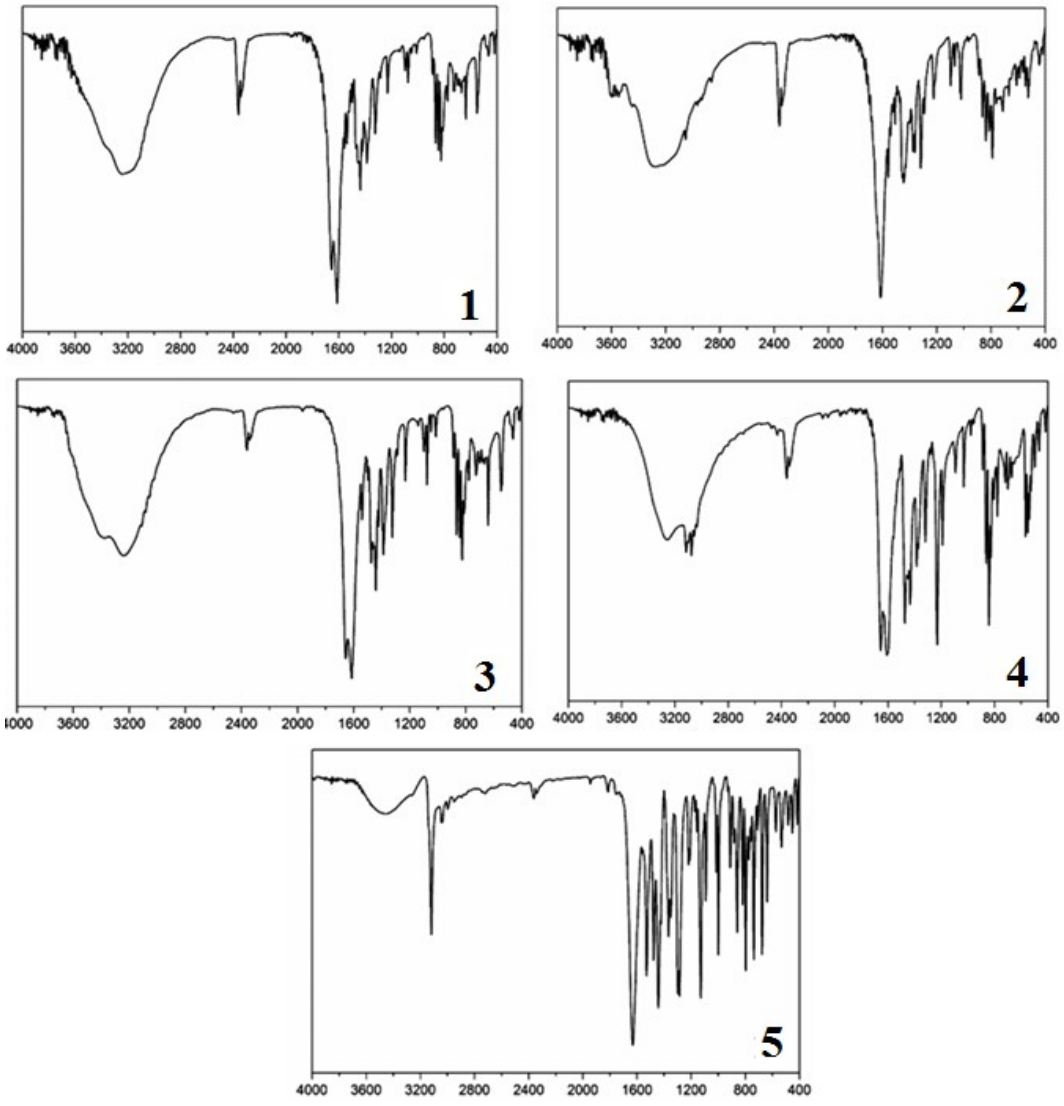

Figure S2. IR spectra of **1**-**5** (4000-400 cm^{-1}).