# Supporting Information

# A Dynamic Open Framework Exhibiting Guest and/or Temperature Induced Bicycle Pedal Motion in Single-crystal to Single-crystal Transformation

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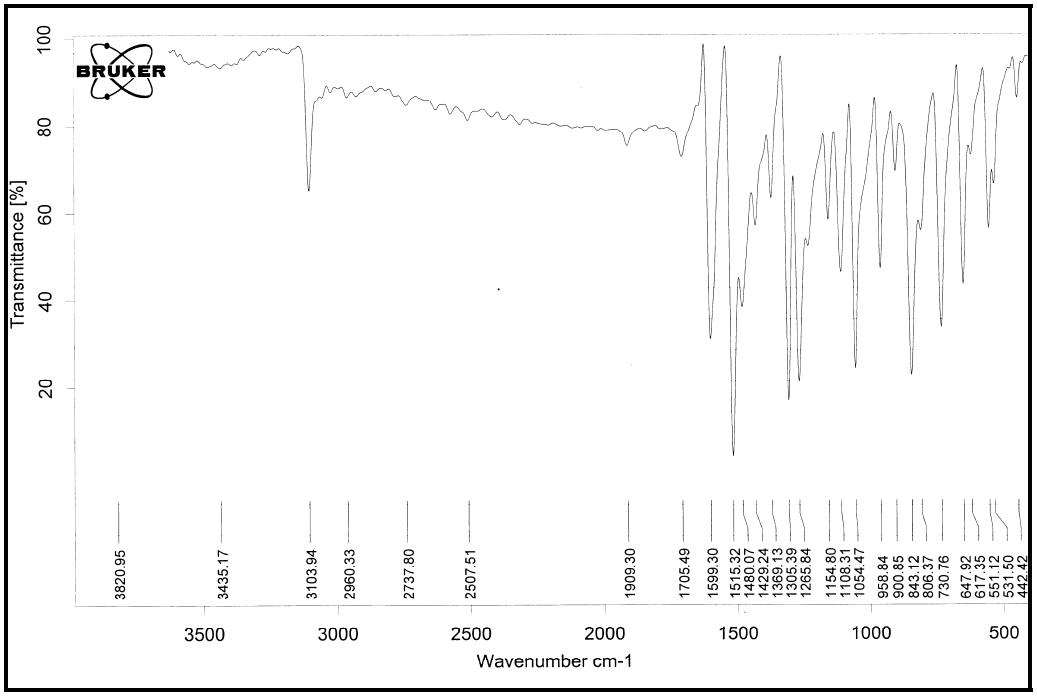


**Figure S1.** FTIR spectrum of ligand azim (bis-(4-imidazol-1-yl-phenyl)-diazene).

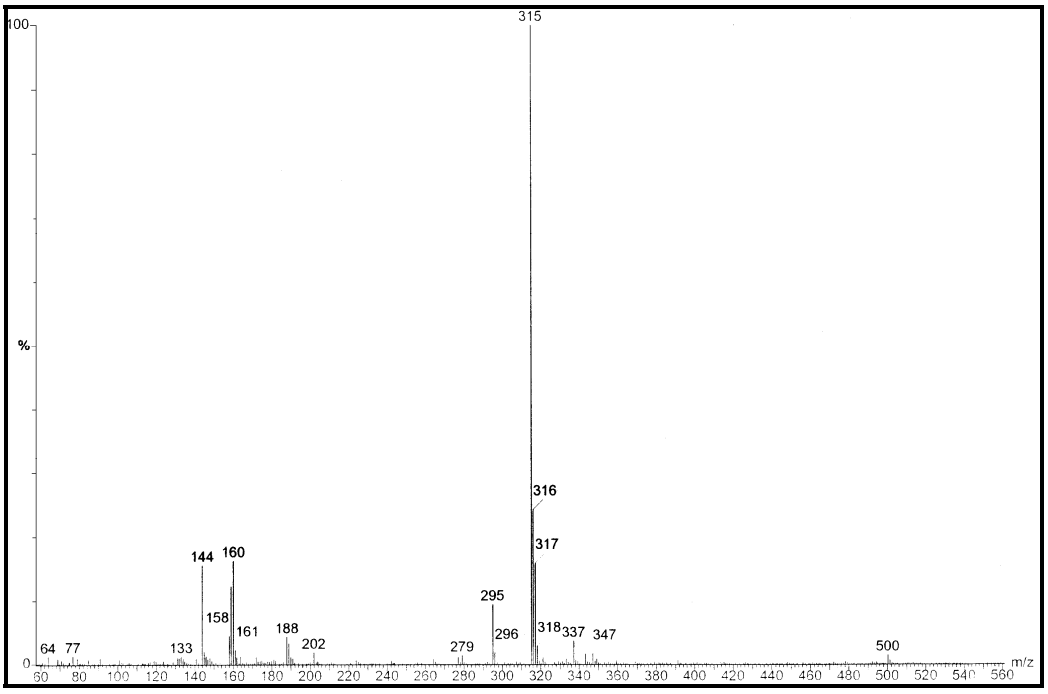


**Figure S2.** ESI mass spectrum of ligand azim (bis-(4-imidazol-1-yl-phenyl)-diazene).

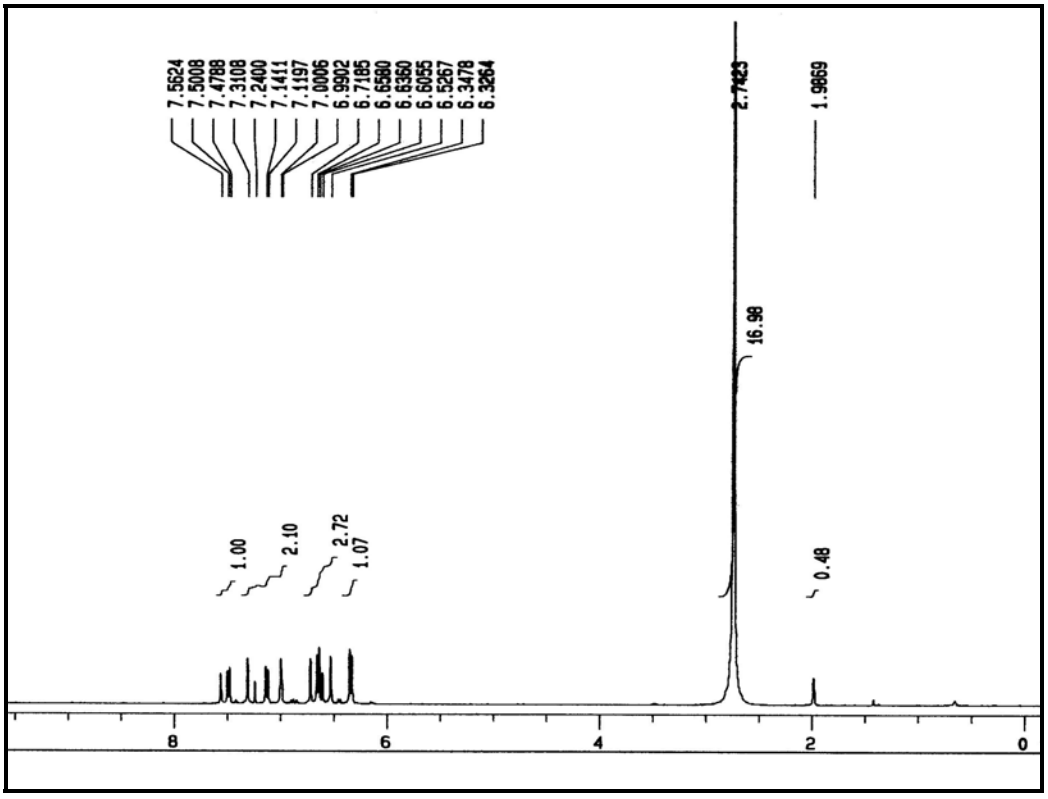


**Figure S3.** $^{1}$H-NMR (400 MHz) of ligand azim **(**bis-(4-imidazol-1-yl-phenyl)-diazene**).**

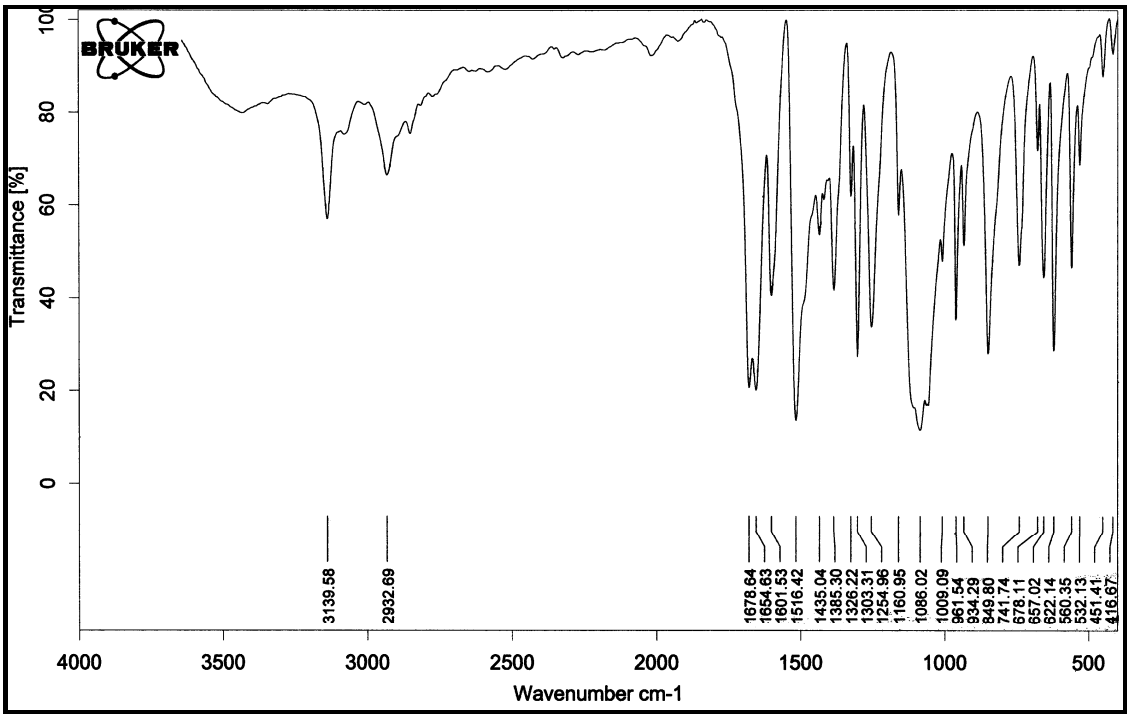


**Figure S4.** FTIR spectrum of as synthesized compound **1**.

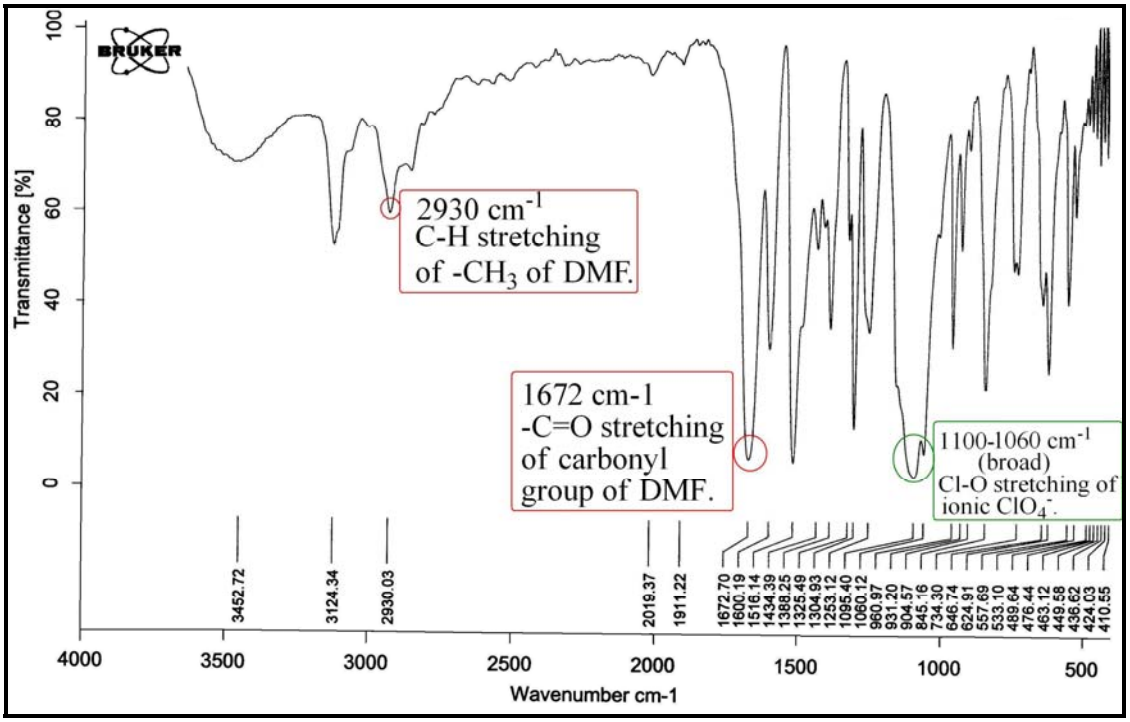


**Figure S5.** FTIR spectrum of as synthesized compound **2**.

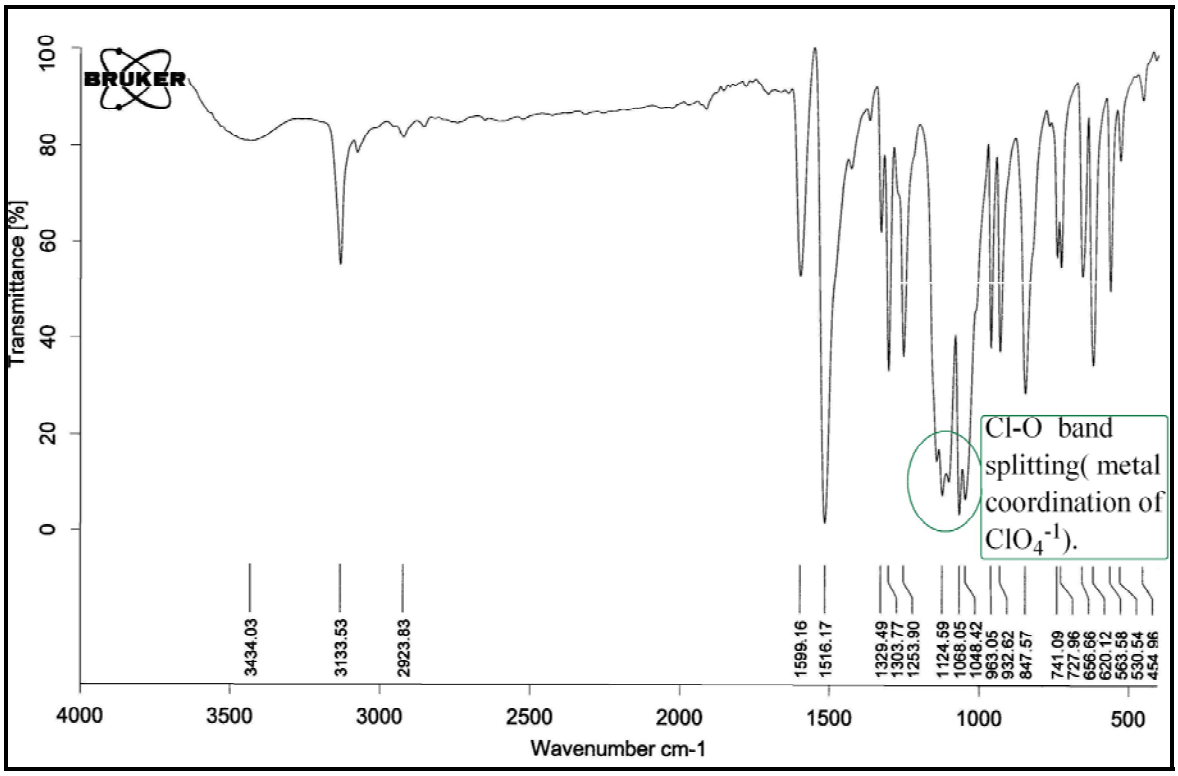


**Figure S6.** FTIR spectrum of compound **2c**.

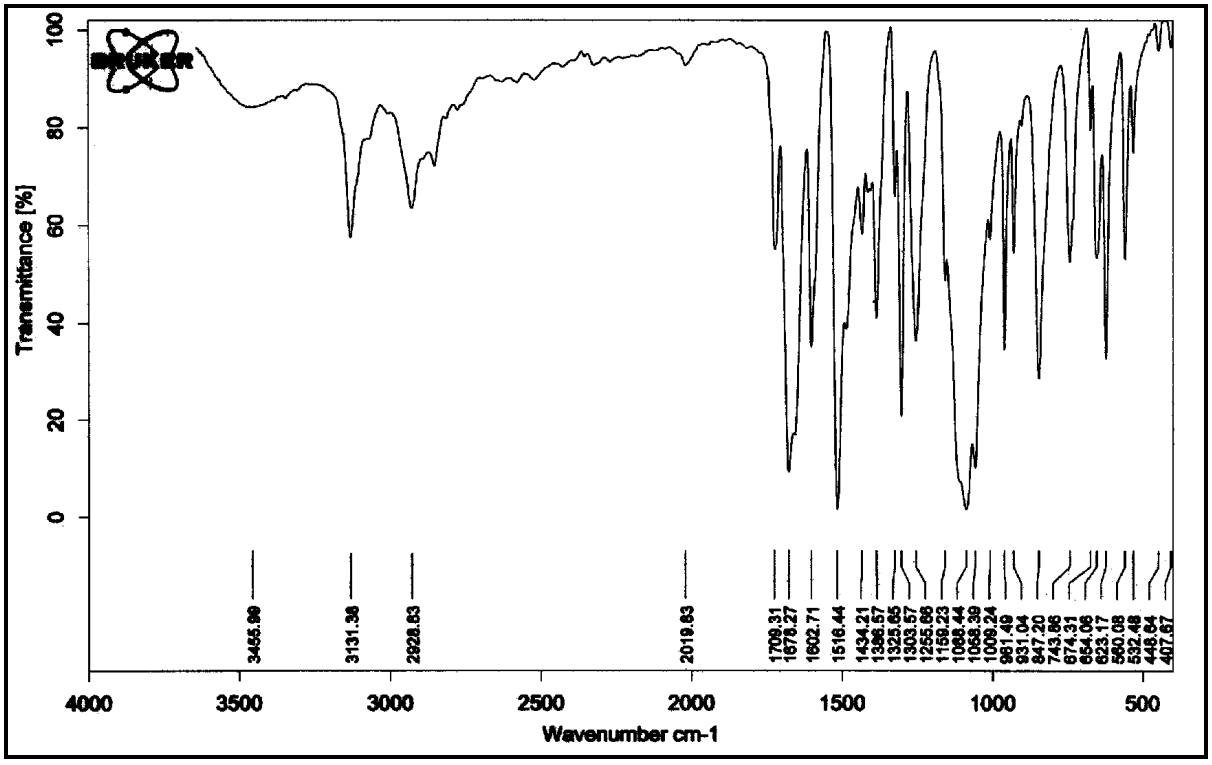


**Figure S7.** FTIR spectrum of compound **3**.

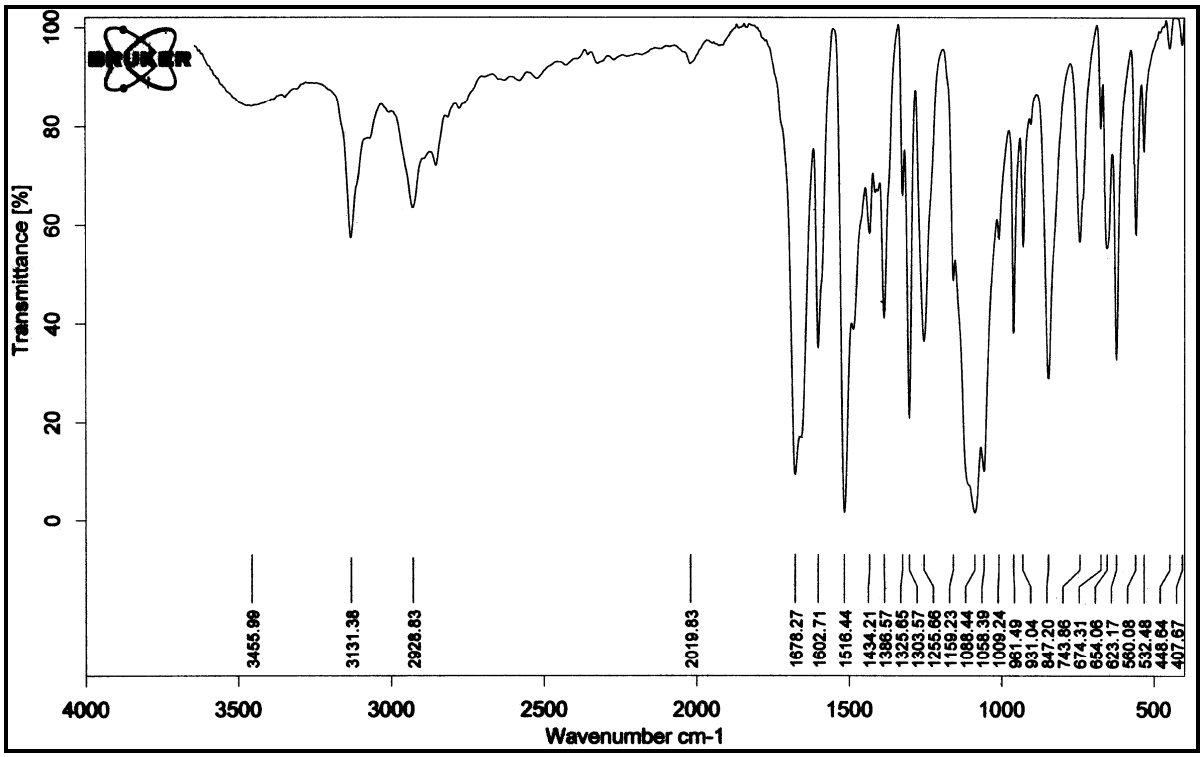


**Figure S8.** FTIR spectrum of compound **4**.

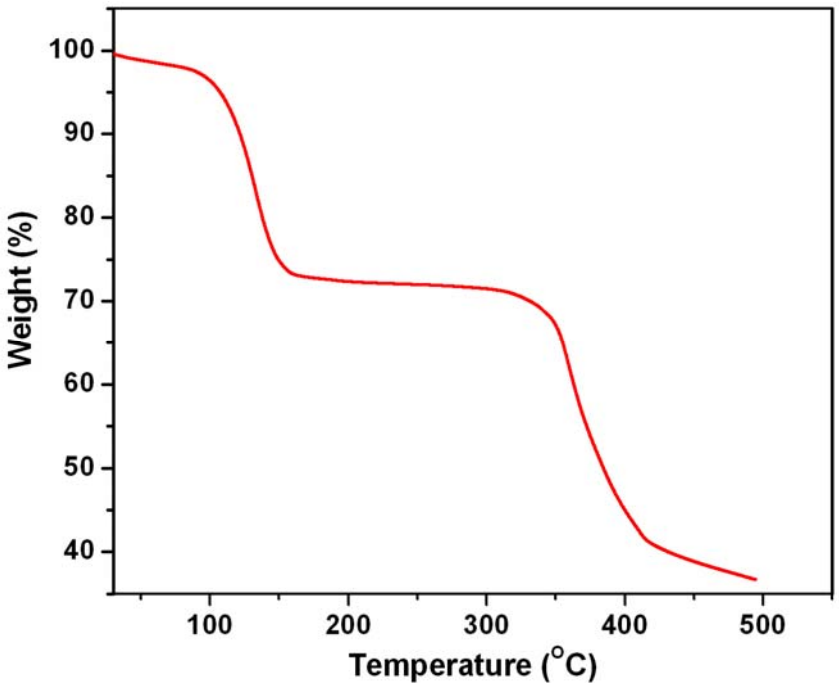


**Figure S9.** Thermogram of compound **1**.

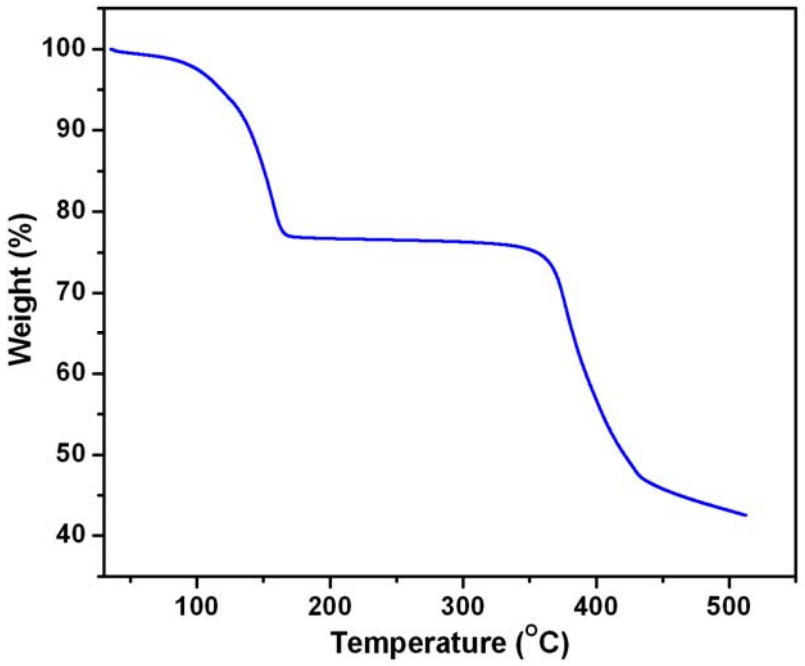


**Figure S10.** Thermogram of compound **2**.

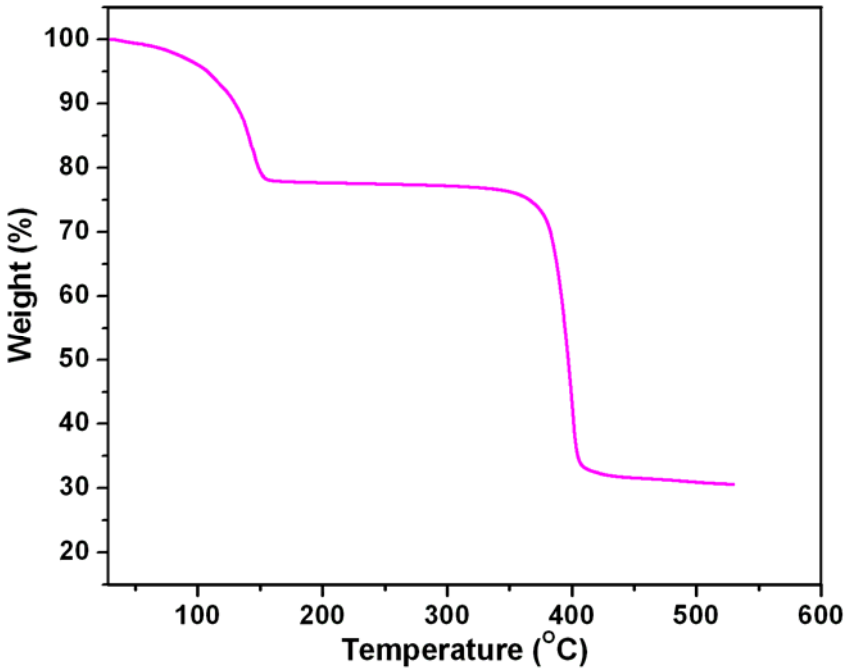


**Figure S11.** Thermogram of compound **3**.

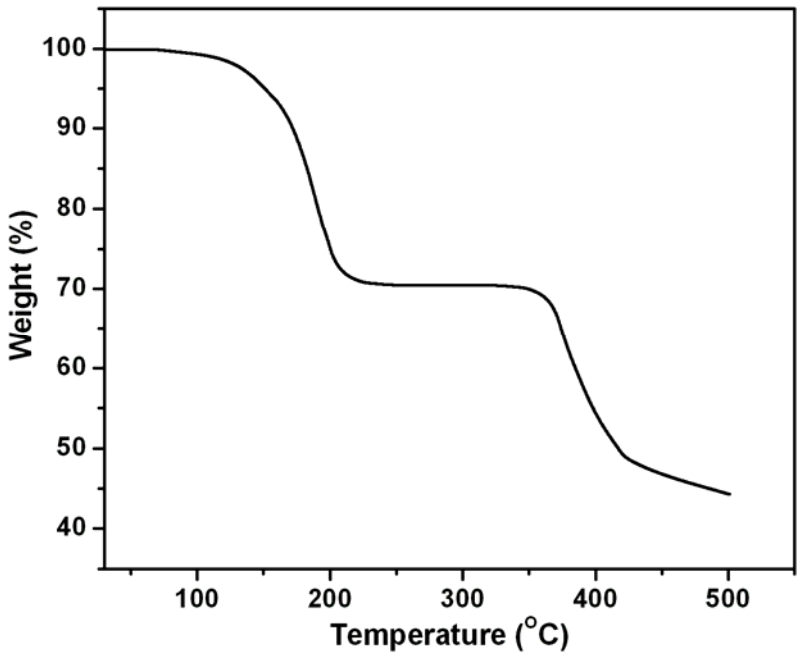


**Figure S12.** Thermogram of compound **4**.

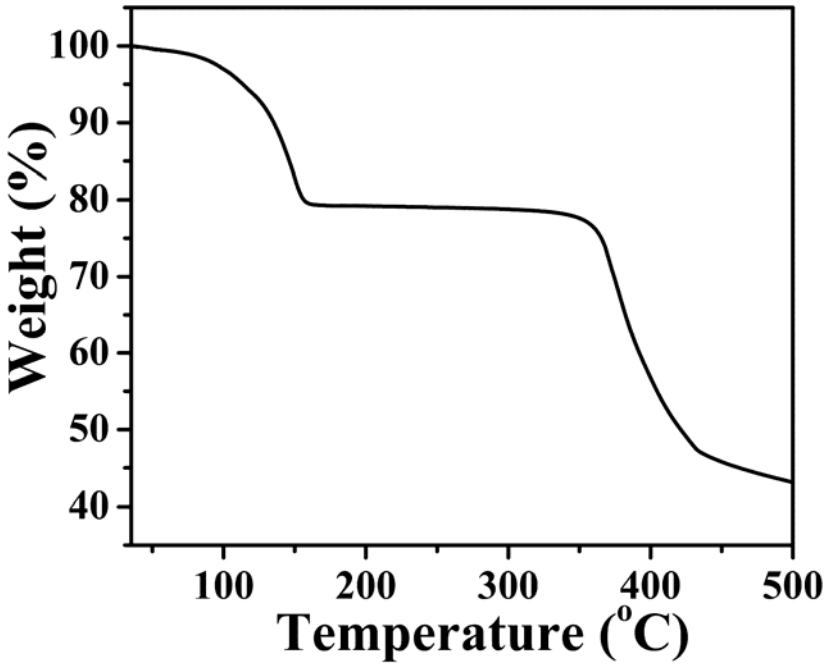


**Figure S13**. Thermogram of compound **2a**.

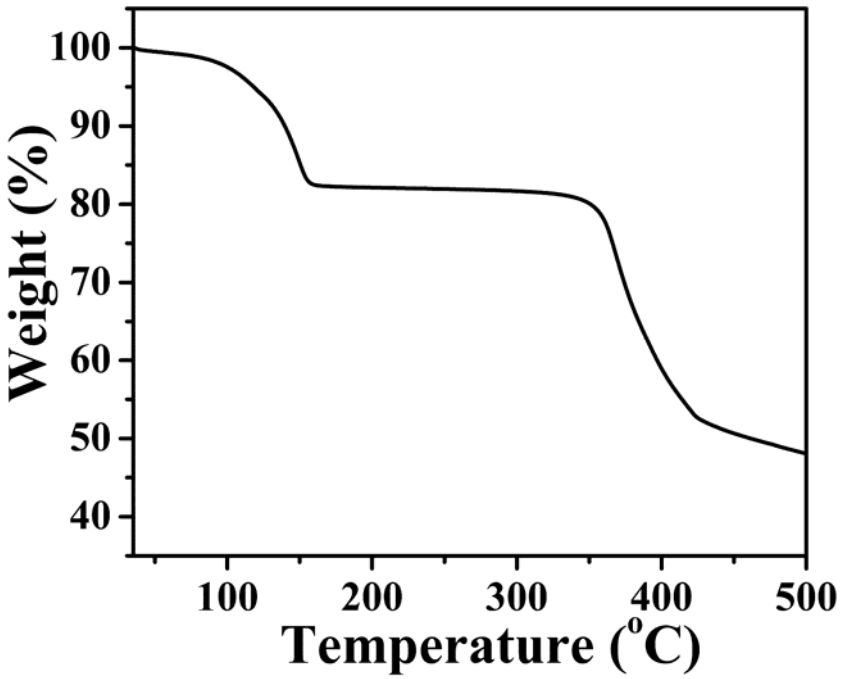


**Figure S14**. Thermogram of compound **2b**.

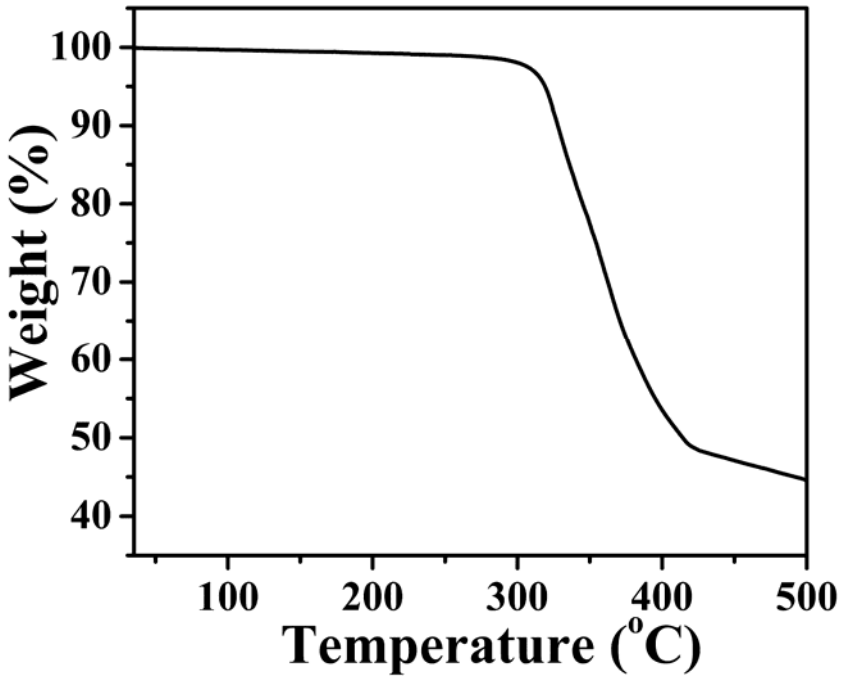


**Figure S15**. Thermogram of compound **2c**.

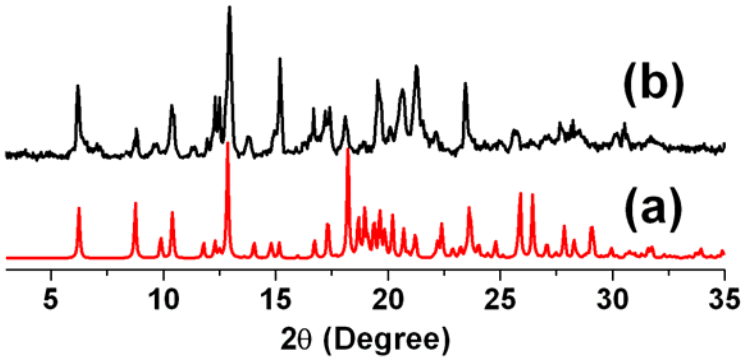


**Figure S16.** PXRD patterns of (a) simulated pattern of **1**. (b) experimental pattern of **1**.

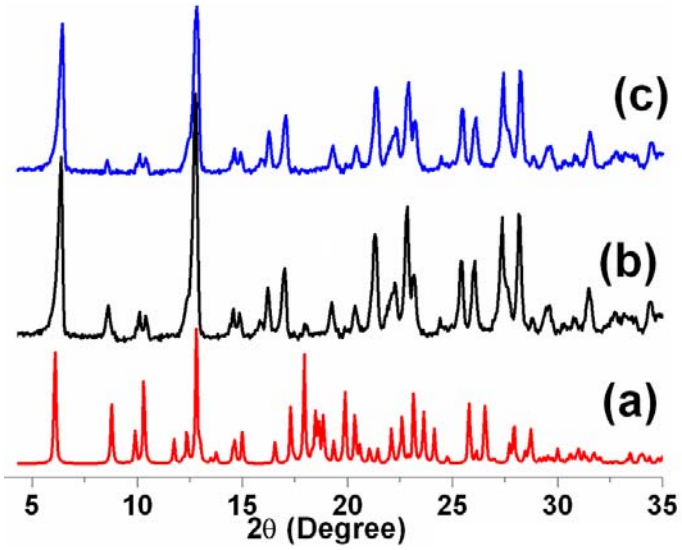


**Figure S17.** PXRD patterns of (a) simulated pattern of **2**. (b) experimental pattern of **2**. (c) experimental pattern of **2′**.

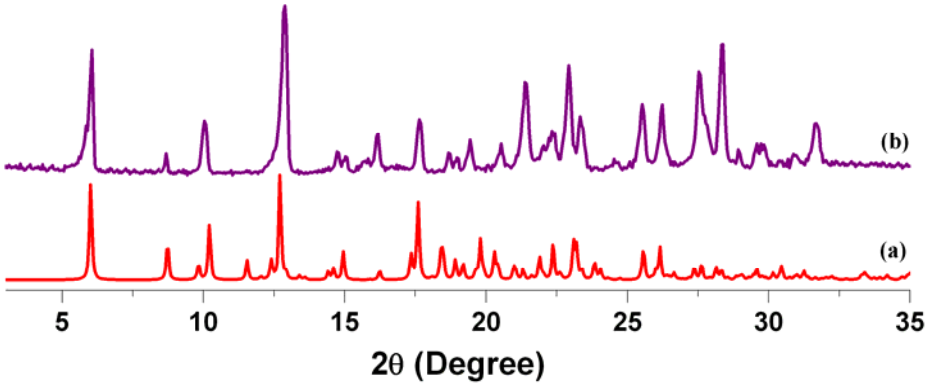


**Figure S18.** PXRD patterns of (a) simulated pattern of **3**. (b) experimental pattern of **3**.

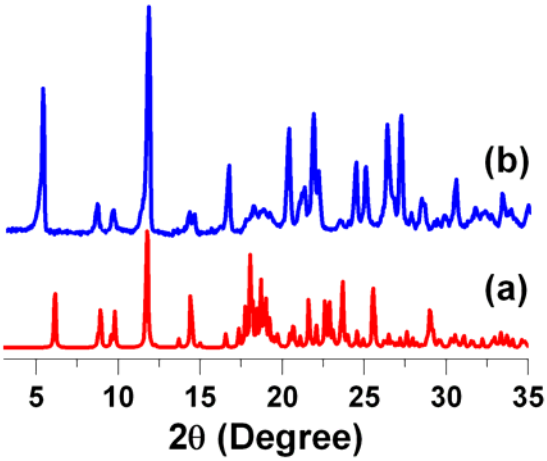


**Figure S19.** PXRD patterns of (a) simulated pattern of **4**. (b) experimental pattern of **4**.

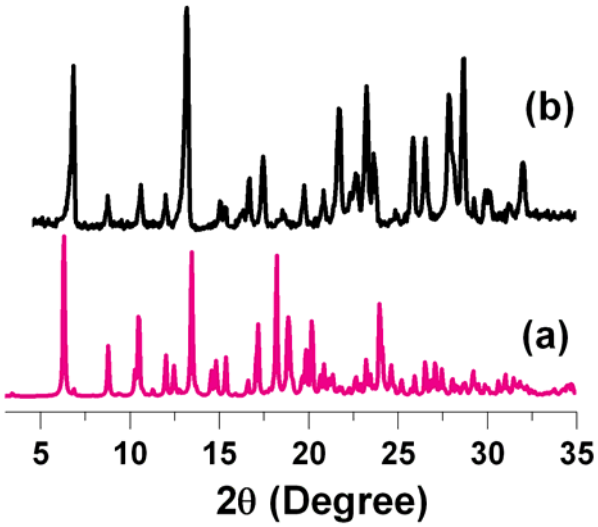


**Figure S20.** PXRD patterns of (a) simulated pattern of **2a**. (b) experimental pattern of **2a**.

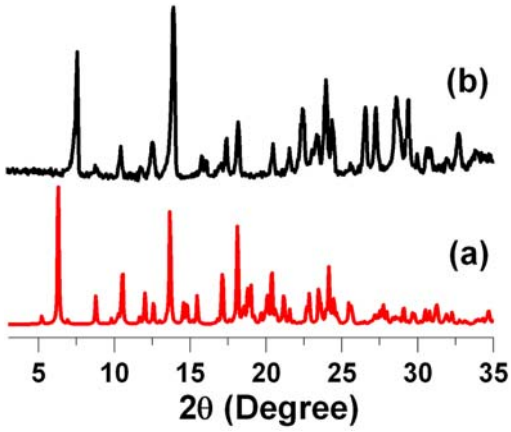


**Figure S21.** PXRD patterns of (a) simulated pattern of **2b**. (b) experimental pattern of **2b**.

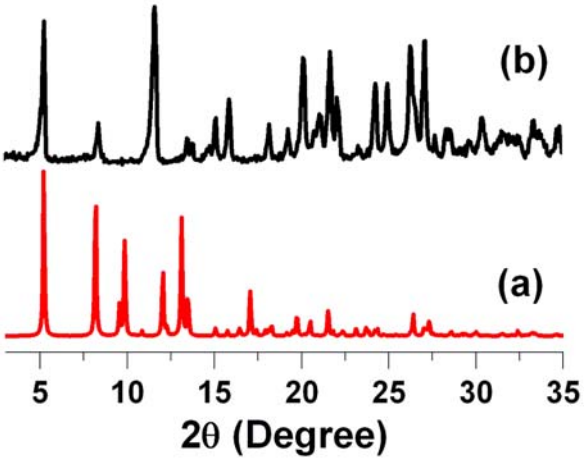


**Figure S22.** PXRD patterns of (a) simulated pattern of **2c**. (b) experimental pattern of **2c**.

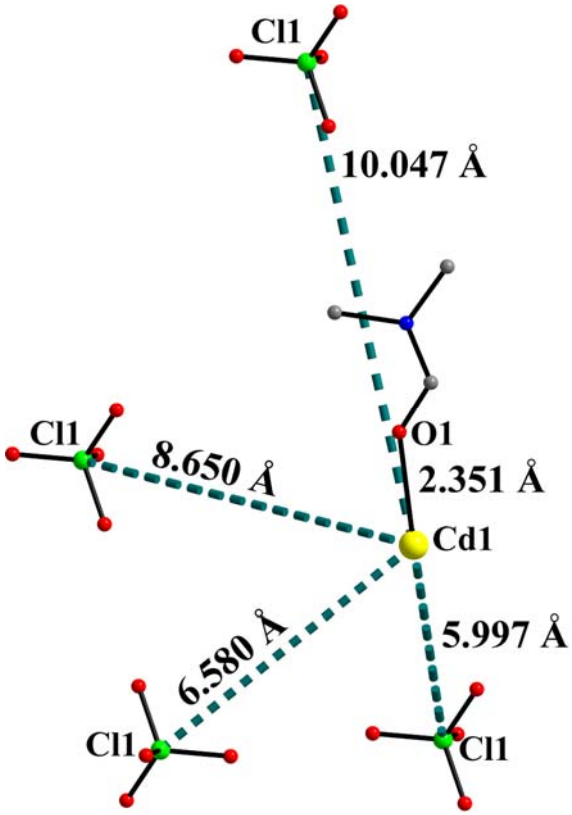


**Figure S23.** Crystal structures of compound **2**, showing the distances between Cd(II) and Cl Atoms of $ClO_4^-$ anions.

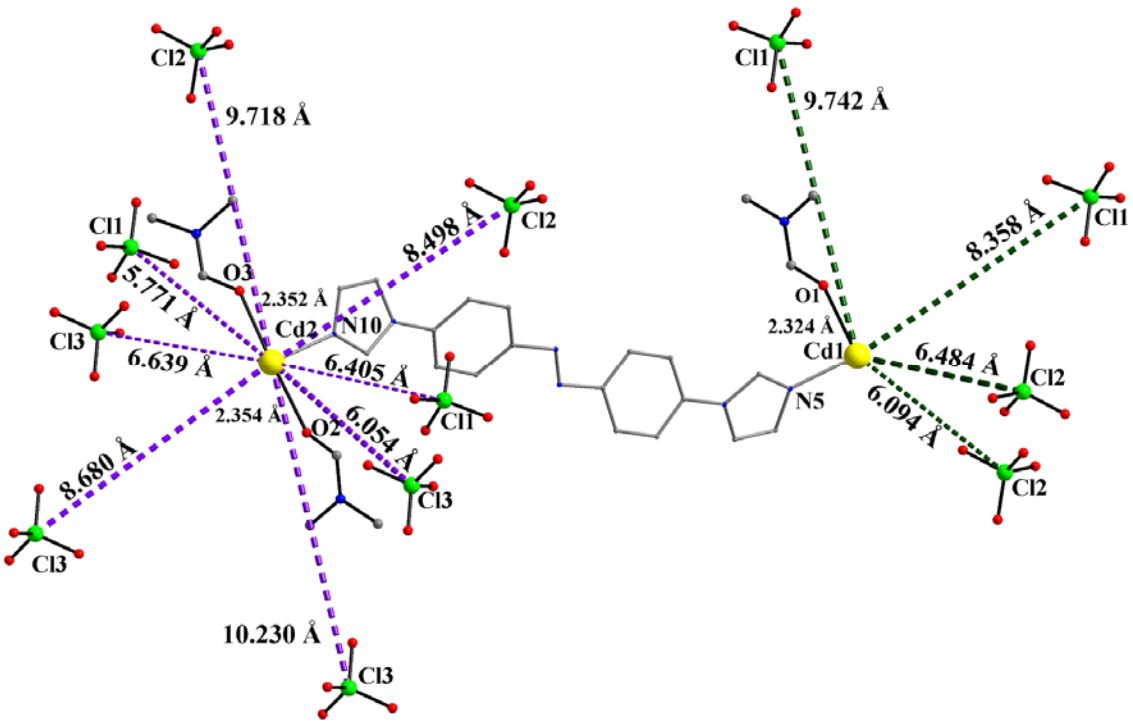


**Figure S24.** Crystal structures of compound **2a**, showing the distances between Cd(II) and Cl Atoms of $ClO_4^-$ anions.

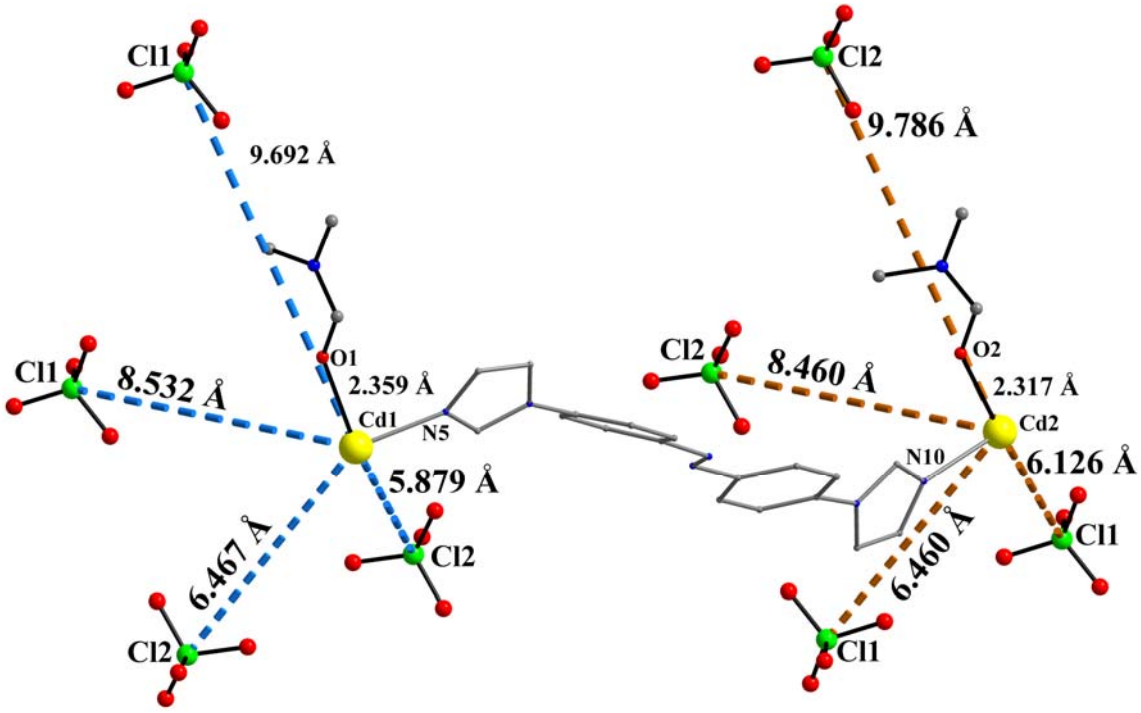


**Figure S25**. Crystal structures of compound **2b**, showing the distances between Cd(II) and Cl Atoms of $ClO_4^-$ anions.

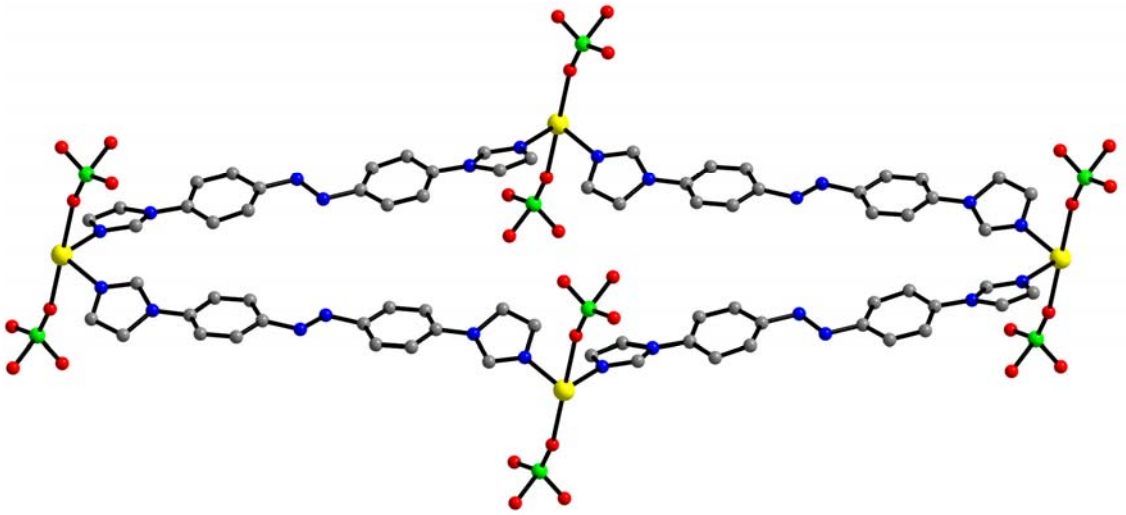

**Figure S26.** A view of coordination of perchlorate anion to the Cd(II) ion in **2c**.

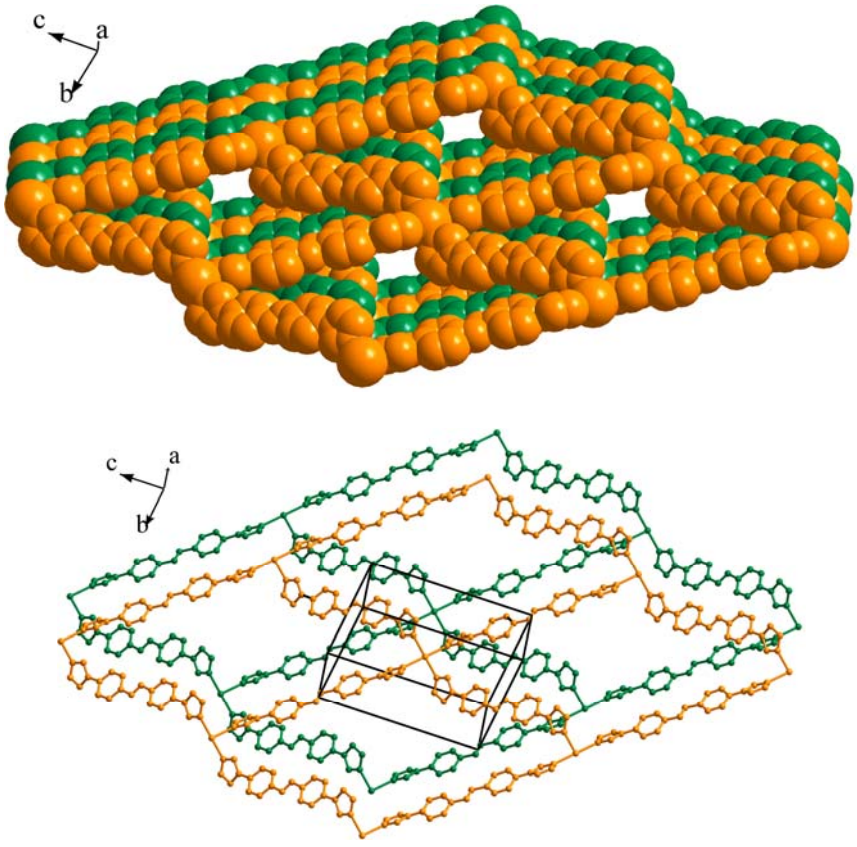


**Figure S27.** A view of **1** (top) showing ABAB….stacking mode of grid layers (CPK model). 2D rhombus grid networks of **1** (bottom) with cell edges (guest molecules are removed for clarity).

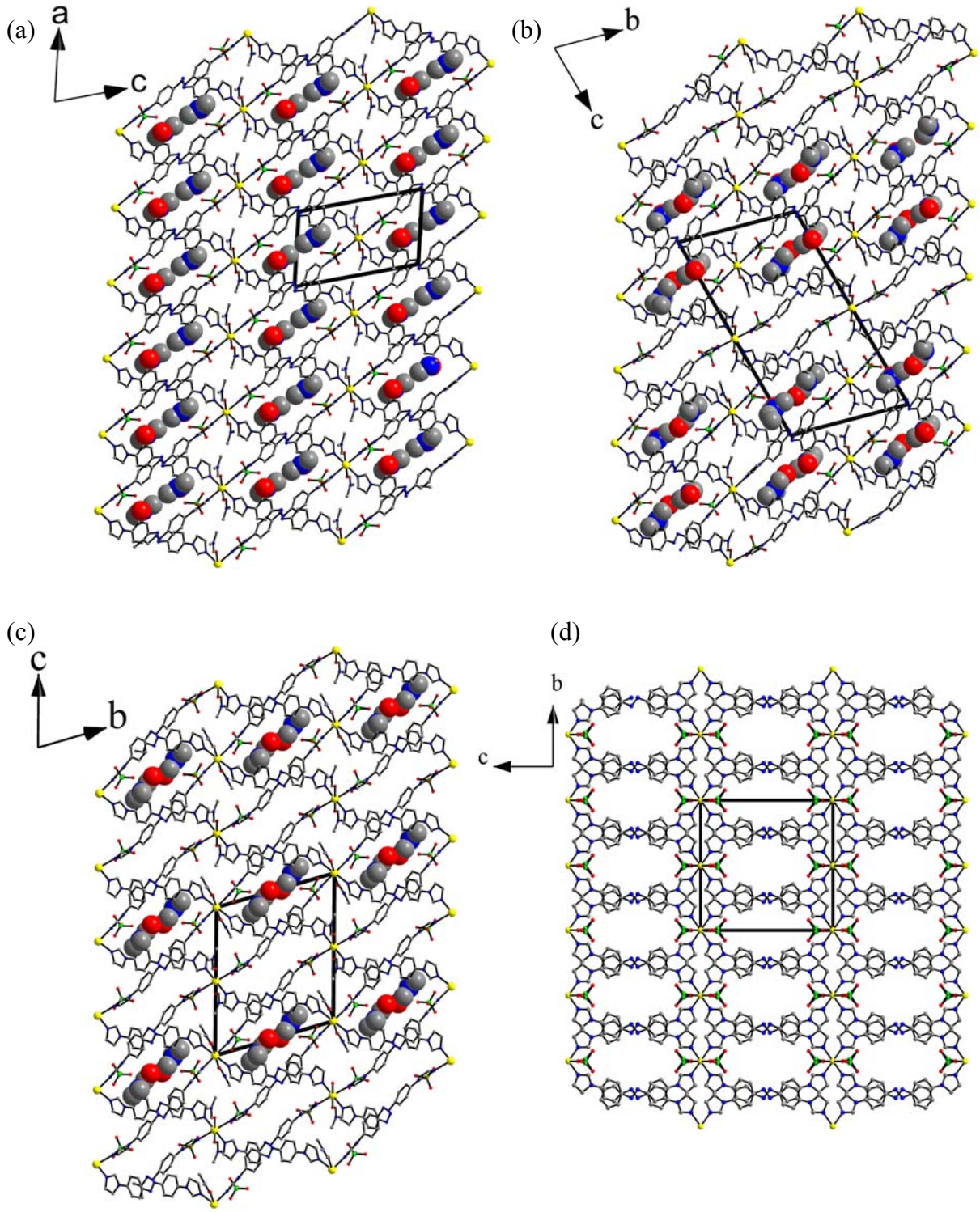


**Figure S28.** Crystal structure of **2** (a), **2a** (b), **2b**(c) and **2c** (d). Cd, pale yellow; O, red; N, blue; C, gray; Cl; green; (grid networks in stick mode showing guest DMF molecules in space-filling mode)

**Table S1.** Selected Bond Distances (Å) and Bond Angles ( $^{o}$ ) in **1**.

| | | |
|---|---|---|
| Bond Distances (Å) | | |
| Co1─ N1 2.125(3) | Co1─N4 2.129(3) | Co1─ O1 2.167(2) |
| Bond Angles ( $^{o}$ ) | | |
| N1 Co1 N4 87.07(11) | N1 Co1 O1 89.48(11) | N4 Co1 O1 84.26(10) |

**Table S2.** Selected Bond Distances (Å) and Bond Angles ( $^{o}$ ) in **2**

| | | | | | |
|---|---|---|---|---|---|
| Bond Distances (Å) | | | | | |
| Cd1—N1 | 2.307(4) | Cd1—N4 | 2.307(4) | Cd1—O1 | 2.351(3) |
| Bond Angles ( $^{o}$ ) | | | | | |
| N1 Cd1 N4 86.66(14) | | N1 Cd1 O1 88.10(14)) | | N4 Cd1 O1 83.21(13) | |

**Table S3.** Selected Bond Distances (Å) and Bond Angles ( $^{o}$ ) in **3**

| | | | | | |
|---|---|---|---|---|---|
| Bond Distances (Å) | | | | | |
| Cd1—N1 | 2.320(5) | Cd1—N4 | 2.313(6) | Cd1—O1 | 2.341(6) |
| Bond Angles ( $^{o}$ ) | | | | | |
| N1 Cd1 N4 86.6(2) | | N1 Cd1 O1 88.0(2) | | N4 Cd1 O1 84.1(2) | |

**Table S4.** Selected Bond Distances (Å) and Bond Angles ( $^{o}$ ) in **4**

| | | | | | |
|---|---|---|---|---|---|
| Bond Distances (Å) | | | | | |
| Cd1—N1 | 2.374(4) | Cd1—N4 | 2.300(4) | Cd1—O1 | 2.332(3) |
| Bond Angles ( $^{o}$ ) | | | | | |
| N1 Cd1 N4 86.69(14) | | N1 Cd1 O1 83.48(13) | | N4 Cd1 O1 84.40(13) | |

**Table S5.** Selected Bond Distances (Å) and Bond Angles ( $^{o}$ ) in **2´**

| | | | | | |
|---|---|---|---|---|---|
| Bond Distances (Å) | | | | | |
| Cd1—N1 | 2.317(4) | Cd1—N4 | 2.322(5) | Cd1—O1 | 2.339(5) |
| Bond Angles ( $^{o}$ ) | | | | | |
| N1 Cd1 N4 | 86.65(18) | N1 Cd1 O1 | 84.85(19) | N4 Cd1 O1 | 87.95(19) |

**Table S6.** Selected Bond Distances (Å) and Bond Angles ( $^{o}$ ) in **2a**

| | | | | | |
|---|---|---|---|---|---|
| Bond Distances (Å) | | | | | |
| Cd1—N1 | 2.343(5) | Cd1—N5 | 2.301(5) | Cd1—O1 | 2.323(4) |
| Cd2—N16 | 2.304(5) | Cd2—N10 | 2.322(5) | Cd2—N14 | 2.326(5) |
| Cd2—N11 | 2.336(5) | Cd2—O2 | 2.353(4) | Cd2—O3 | 2.352(4) |
| Bond Angles ( $^{o}$ ) | | | | | |
| N5 Cd1 N5 | 180.000(1) | N5 Cd1 O1 | 89.72(16) | N5 Cd1 O1 | 90.28(16) |
| N5 Cd1 O1 | 90.28(16) | N5 Cd1 O1 | 89.72(16) | O1 Cd1 O1 | 180.00(18) |
| N5 Cd1 N1 | 90.14(17) | N5 Cd1 N1 | 89.86(17) | O1 Cd1 N1 | 82.57(16) |
| O1 Cd1 N1 | 97.43(16) | N5 Cd1 N1 | 89.86(17) | N5 Cd1 N1 | 90.14(17) |
| O1 Cd1 N1 | 97.43(16) | O1 Cd1 N1 | 82.57(16) | N1 Cd1 N1 | 180.000(1) |
| N16 Cd2 N10 | 177.00(16) | N16 Cd2 N14 | 94.23(16) | N10 Cd2 N14 | 88.77(16) |
| N16 Cd2 N11 | 86.91(16) | N10 Cd2 N11 | 90.09(16) | N14 Cd2 N11 | 178.86(16) |
| N16 Cd2 O3 | 94.86(15) | N10 Cd2 O3 | 85.25(16) | N14 Cd2 O3 | 85.05(15) |
| N11 Cd2 O3 | 94.88(16) | N16 Cd2 O2 | 88.68(16) | N10 Cd2 O2 | 91.09(16) |
| N14 Cd2 O2 | 97.19(15) | N11 Cd2 O2 | 82.80(16) | O3 Cd2 O2 | 175.67(14) |

**Table S7.** Selected Bond Distances (Å) and Bond Angles ( $^{o}$ ) in **2b**

| | | |
|---|---|---|
| Bond Distances (Å) | | |
| Cd1—N5 2.315(6) | Cd1—N1 2.336(7) | Cd1—O1 2.363(6) |
| Cd2—N11 2.297(7) | Cd2—O2 2.318(6) | Cd2—N10 2.349(7) |
| Bond Angles ( $^{o}$ ) | | |
| N5 Cd1 N5 180.0(5) | N5 Cd1 N1 88.2(2) | N5 Cd1 N1 91.8(2) |
| N1 Cd1 N1 180.0(5) | N5 Cd1 O1 85.6(2) | N5 Cd1 O1 94.4(2) |
| N1 Cd1 O1 84.9(2) | N1 Cd1 O1 95.1(2) | O1 Cd1 O1 180.0(3) |
| N11 Cd2 N11 180.0(3) | N11 Cd2 O2 90.4(2) | N11 Cd2 O2 89.6(2) |
| O2 Cd2 O2 180.000(1) | N11 Cd2 N10 90.0(2) | O2 Cd2 N10 97.3(2) |
| O2 Cd2 N10 82.7(2) | O2 Cd2 N10 82.7(2) | N10 Cd2 N10 180.000(1) |

**Table S8.** Selected Bond Distances (Å) and Bond Angles ( $^{o}$ ) in **2c**

| | | |
|---|---|---|
| Bond Distances (Å) | | |
| Cd1—N1 2.229(16) | Cd1—O1 2.478(14) | |
| Bond Angles ( $^{o}$ ) | | |
| N1 Cd1 N1 180.000(1) | N1 Cd1 N1 80.2(10) | N1 Cd1 N1 99.8(10) |
| N1 Cd1 O1 90.0(11) | | |