Electronic supporting information (ESI)

# Two three-dimensional cadmium(II) coordination polymers based on 5-amino-tetrazolate and 1,2,4,5-benzenetetracarboxylate: pH value controlled syntheses, crystal structures, and luminescent properties

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**Table S1.** Selected Bond Lengths (Å) and Angles (˚) for **1** and **2**[a]

| | | | | | |
|---|---|---|---|---|---|
| **CP 1** | | | | | |
| Cd(1)-N(2) | 2.210(4) | Cd(1)-O(2) | 2.292(3) | Cd(1)-O(3B) | 2.387(3) |
| Cd(1)-O(4A) | 2.243(3) | Cd(1)-O(1W) | 2.312(4) | Cd(1)-O(1) | 2.429(3) |
| N(2)-Cd(1)-O(4A) | 98.05(12) | O(2)-Cd(1)-O(1W) | 87.00(16) | N(2)-Cd(1)-O(1) | 106.55(11) |
| N(2)-Cd(1)-O(2) | 162.26(11) | N(2)-Cd(1)-O(3B) | 87.46(12) | O(4A)-Cd(1)-O(1) | 153.96(11) |
| O(4A)-Cd(1)-O(2) | 99.29(11) | O(4A)-Cd(1)-O(3B) | 74.98(10) | O(2)-Cd(1)-O(1) | 55.75(10) |
| N(2)-Cd(1)-O(1W) | 93.81(17) | O(2)-Cd(1)-O(3B) | 93.41(11) | O(1W)-Cd(1)-O(1) | 87.32(15) |
| O(4A)-Cd(1)-O(1W) | 99.61(14) | O(1W)-Cd(1)-O(3B) | 174.57(14) | O(3B)-Cd(1)-O(1) | 97.39(10) |
| **CP 2** | | | | | |
| Cd(1)-N(5) | 2.250(4) | Cd(2)-O(9) | 2.218(4) | Cd(3)-O(9B) | 2.243(4) |
| Cd(1)-O(8A) | 2.255(4) | Cd(2)-N(2C) | 2.291(4) | Cd(3)-O(9F) | 2.294(3) |
| Cd(1)-O(1) | 2.348(3) | Cd(2)-O(6D) | 2.296(3) | Cd(3)-O(4B) | 2.295(4) |
| Cd(1)-O(5B) | 2.367(4) | Cd(2)-O(1W) | 2.357(4) | Cd(3)-O(2W) | 2.319(4) |
| Cd(1)-O(7B) | 2.400(4) | Cd(2)-O(1) | 2.420(3) | Cd(3)-O(3G) | 2.345(4) |
| Cd(1)-O(2) | 2.490(3) | Cd(2)-O(3E) | 2.454(4) | Cd(3)-N(3) | 2.392(5) |
| N(5)-Cd(1)-O(8A) | 108.58(15) | O(9)-Cd(2)-N(2C) | 94.25(15) | O(9B)-Cd(3)-O(9F) | 82.37(14) |
| N(5)-Cd(1)-O(1) | 128.98(15) | O(9)-Cd(2)-O(6D) | 97.22(14) | O(9B)-Cd(3)-O(4B) | 100.78(13) |
| O(8A)-Cd(1)-O(1) | 95.47(13) | N(2C)-Cd(2)-O(6D) | 159.60(14) | O(9F)-Cd(3)-O(4B) | 166.41(15) |
| N(5)-Cd(1)-O(5B) | 87.81(14) | O(9)-Cd(2)-O(1W) | 175.30(13) | O(9B)-Cd(3)-O(2W) | 172.50(16) |
| O(8A)-Cd(1)-O(5B) | 160.28(12) | N(2C)-Cd(2)-O(1W) | 86.95(15) | O(9F)-Cd(3)-O(2W) | 91.73(15) |
| O(1)-Cd(1)-O(5B) | 81.73(12) | O(6D)-Cd(2)-O(1W) | 80.33(13) | O(4B)-Cd(3)-O(2W) | 86.03(15) |
| N(5)-Cd(1)-O(7B) | 99.39(14) | O(9)-Cd(2)-O(1) | 93.00(13) | O(9B)-Cd(3)-O(3G) | 95.90(13) |
| O(8A)-Cd(1)-O(7B) | 90.26(13) | N(2C)-Cd(2)-O(1) | 91.04(13) | O(9F)-Cd(3)-O(3G) | 73.71(13) |
| O(1)-Cd(1)-O(7B) | 125.46(12) | O(6D)-Cd(2)-O(1) | 71.61(12) | O(4B)-Cd(3)-O(3G) | 92.77(13) |
| O(5B)-Cd(1)-O(7B) | 75.93(13) | O(1W)-Cd(2)-O(1) | 82.43(13) | O(2W)-Cd(3)-O(3G) | 86.83(16) |
| N(5)-Cd(1)-O(2) | 166.08(14) | O(9)-Cd(2)-O(3E) | 72.91(13) | O(9B)-Cd(3)-N(3) | 89.25(14) |
| O(8A)-Cd(1)-O(2) | 83.30(12) | N(2C)-Cd(2)-O(3E) | 82.47(13) | O(9F)6-Cd(3)-N(3) | 100.86(14) |
| O(1)-Cd(1)-O(2) | 54.39(12) | O(6D)-Cd(2)-O(3E) | 117.03(11) | O(4B)-Cd(3)-N(3) | 92.43(14) |
| O(5B)-Cd(1)-O(2) | 79.22(12) | O(1W)-Cd(2)-O(3E) | 111.77(13) | O(2W)-Cd(3)-N(3) | 87.31(17) |
| O(7B)-Cd(1)-O(2) | 72.72(11) | O(1)-Cd(2)-O(3E) | 163.89(13) | O(3G)-Cd(3)-N(3) | 171.88(14) |

[a] Symmetry transformations used to generate equivalent atoms: A -*x*, -*y*+1, -*z*; B -*x*, *y*, -*z*+1/2 for **1**.

A -*x*+1, -*y*, -*z*; B *x*, *y*+1, *z*; C *x*, *y*-1, *z*; D *x*-1, *y*+1, *z*; E *x*-1, *y*, *z*; F -*x*, -*y*+1, -*z*+1; G -*x*+1, -*y*+1, -*z*+1 for **2**.

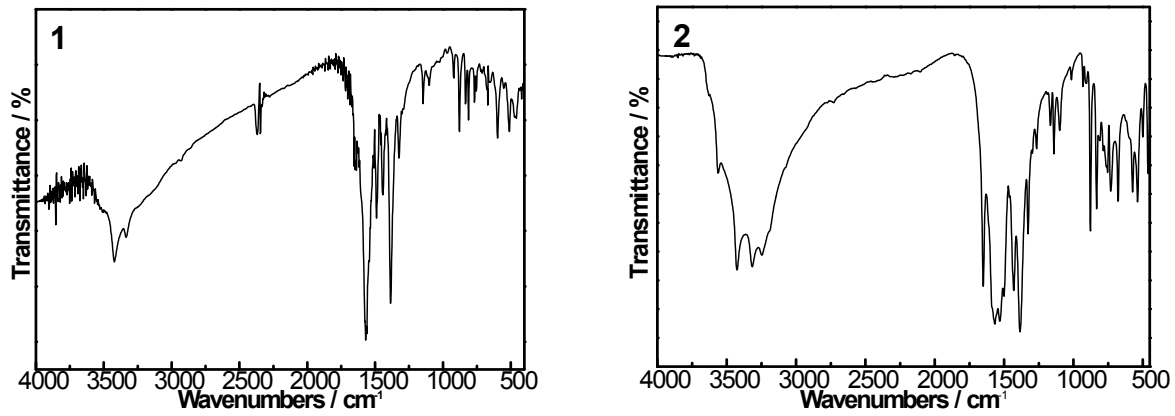


**Fig. S1.** IR spectra of **1** and **2**

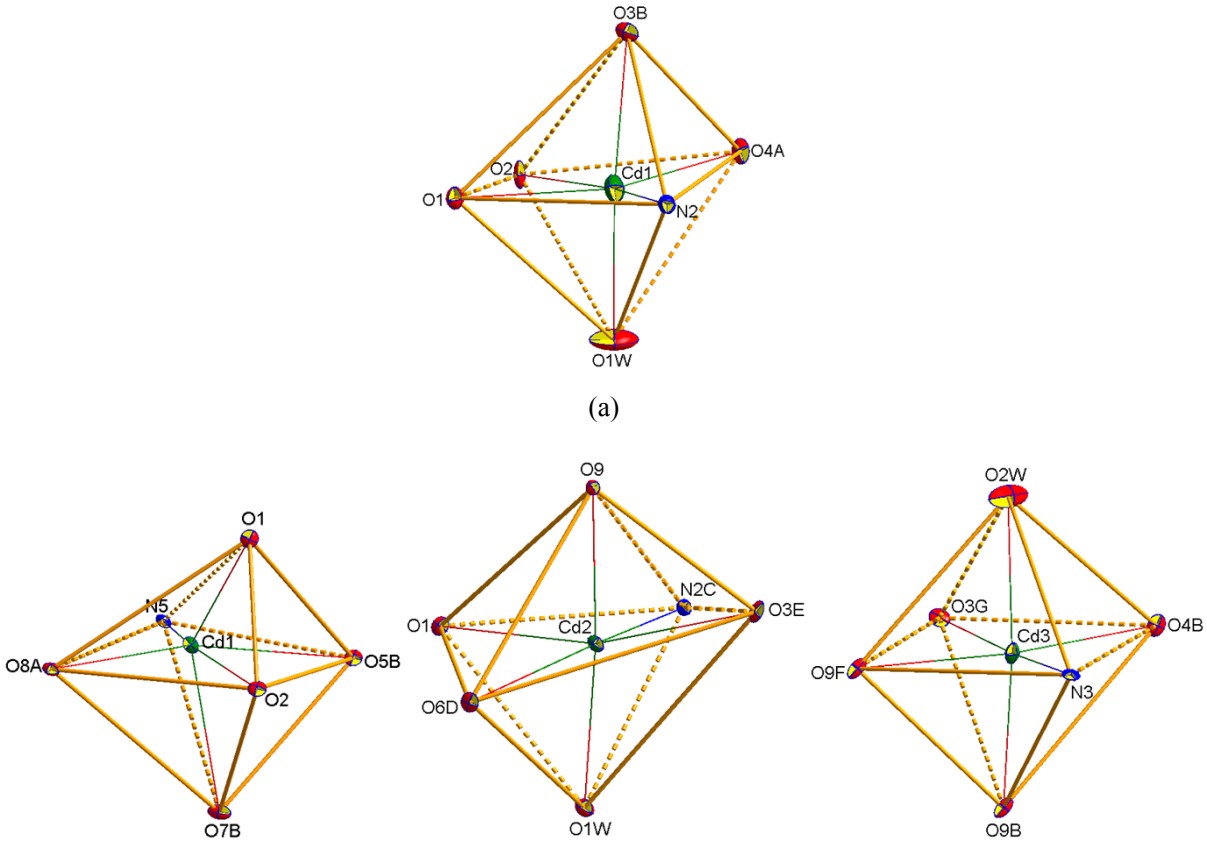


**Fig. S2** The coordination polyhedra of Cd(II) ions in **1** (a) and **2** (b, c, and d).

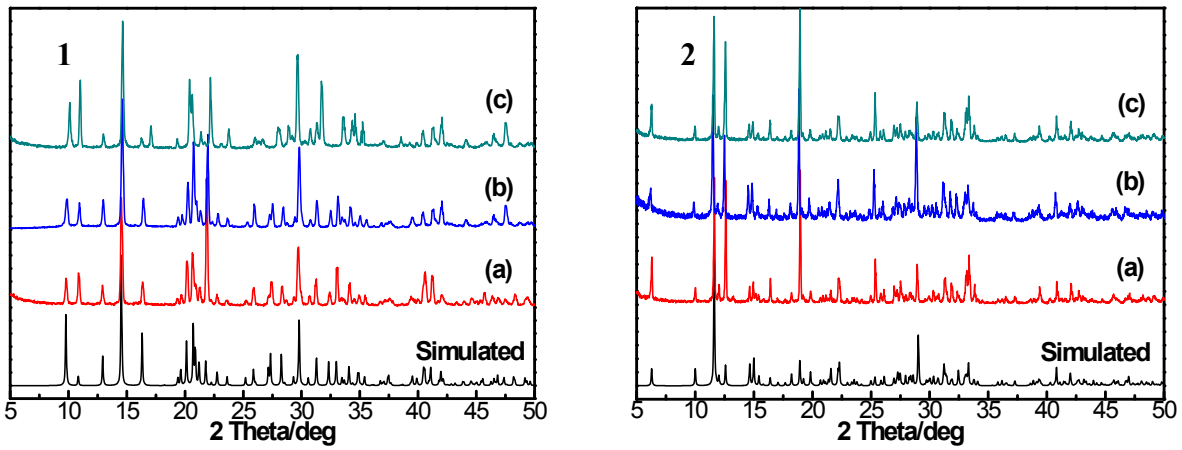


**Fig. S3.** The powder X-ray diffraction patterns for **1** and **2**, the bulk of samples were synthesized from (a) $Cd(NO_3)_2$, (b) $CdCl_2$, and (c) $Cd(Ac)_2$ (the simulated PXRD patterns are generated from the corresponding single-crystal diffraction data).