Electronic Supplementary Information (ESI)

Substituted groups-directed assembly of Cd(II) coordination polymers based on 5-R-1,3-benzenedicarboxylate and 4,4'-bis(1-imidazolyl)bibenzene: syntheses, structures and photoluminescent properties

Hong-Jian Cheng, ^a Hong-Xi Li, ^a Zhi-Gang Ren, ^a Chun-Ning Lü, ^a Jing Shi ^a and Jian-Ping Lang * ^{a,b}

^a Key Laboratory of Organic Synthesis of Jiangsu Province, College of Chemistry, Chemical Engineering and Materials Science, Soochow University, Suzhou 215123, Jiangsu, P. R. China.

^b State Key Laboratory of Organometallic Chemistry, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, Shanghai 200032, P. R. China

Table of Contents

Figure S1. PXRD patterns for **1-6**. (a) simulated (red) and single-phase polycrystalline sample (black) of **1**. (b) simulated (red) and single-phase polycrystalline sample (black) of **2**. (c) simulated (red) and single-phase polycrystalline sample (black) of **3**. (d) simulated (red) and single-phase polycrystalline sample (black) of **4**. (e) simulated (red) and single-phase polycrystalline sample (black) of **5**. (f) simulated (red) and single-phase polycrystalline sample (black) of **6**.......S3

Figure S2. (a) View of the coordination environment of Cd1 in **2**, with a labeling scheme. Symmetry codes: (A) x + 1, y, z + 1.; (B) -x + 1, y + 1/2, -z + 1/2; (C) x, -y + 1/2, z - 1/2. (b) View of a 2D (4, 4) network that is constructed by $[Cd_2(CH_3-1,3-BDC)_4]$ units extending along the bc plane. S4

Figure S3. (a) View of the coordination environment of Cd1 in **3**, with a labeling scheme. Symmetry codes: (A) x + 1, y, z + 1.; (B) -x + 1, y + 1/2, -z + 1/2; (C) x, -y + 1/2, z - 1/2. (b) View of a 2D (4, 4) network that is constructed by $[Cd_2(NH_2-1,3-BDC)_4]$ units extending along the bc plane. S4

Figure S4. (a) View of the coordination environment of Cd1 in **4**, with a labeling scheme. Symmetry codes: (A) x + 1, y, z + 1.; (B) -x + 1, y + 1/2, -z + 1/2; (C) x, -y + 1/2, z - 1/2. (b) View of a 2D (4, 4) network that is constructed by [Cd₂(OH-1,3-BDC)₄] units extending along the bc plane. S5

Figure S5. The TGA curves for 1 (black), 2 (blue), 3 (red), 4 (olive), 5 (magenta) and 6 (purple)......S5

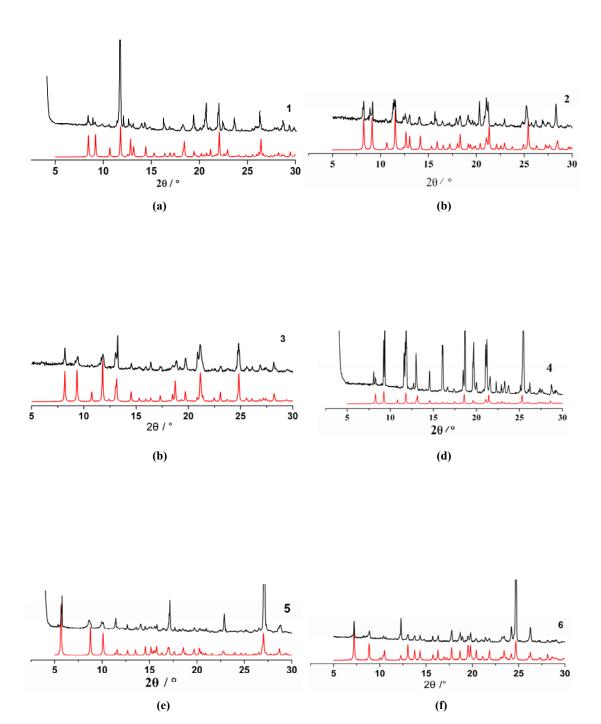


Figure S1. PXRD patterns for **1-6**. (a) simulated (red) and single-phase polycrystalline sample (black) of **1**. (b) simulated (red) and single-phase polycrystalline sample (black) of **2**. (c) simulated (red) and single-phase polycrystalline sample (black) of **3**. (d) simulated (red) and single-phase polycrystalline sample (black) of **4**. (e) simulated (red) and single-phase polycrystalline sample (black) of **5**. (f) simulated (red) and single-phase polycrystalline sample (black) of **6**.

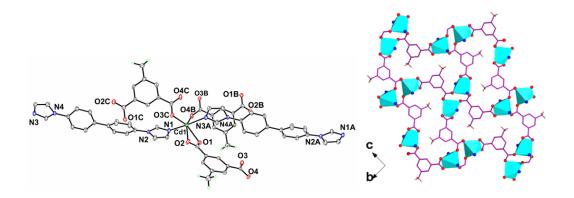


Figure S2. (a) View of the coordination environment of Cd1 in **2**, with a labeling scheme. Symmetry codes: (A) x + 1, y, z + 1.; (B) -x + 1, y + 1/2, -z + 1/2; (C) x, -y + 1/2, z - 1/2. (b) View of a 2D (4, 4) network that is constructed by $[Cd_2(CH_3-1,3-BDC)_4]$ units extending along the bc plane.

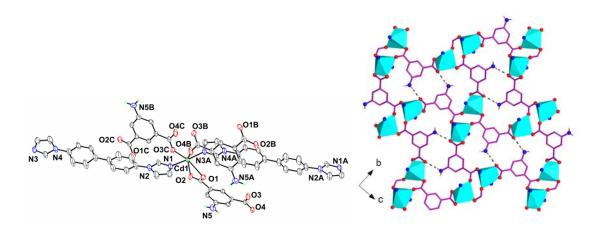


Figure S3. (a) View of the coordination environment of Cd1 in **3**, with a labeling scheme. Symmetry codes: (A) x + 1, y, z + 1.; (B) -x + 1, y + 1/2, -z + 1/2; (C) x, -y + 1/2, z - 1/2. (b) View of a 2D (4, 4) network that is constructed by $[Cd_2(NH_2-1,3-BDC)_4]$ units extending along the bc plane.

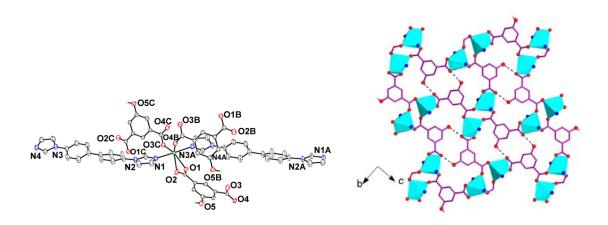


Figure S4. (a) View of the coordination environment of Cd1 in **4**, with a labeling scheme. Symmetry codes: (A) x + 1, y, z + 1; (B) -x + 1, y + 1/2, -z + 1/2; (C) x, -y + 1/2, z - 1/2. (b) View of a 2D (4, 4) network that is constructed by $[Cd_2(HO-1,3-BDC)_4]$ units extending along the bc plane.

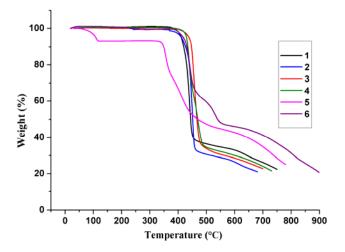


Figure S5. The TGA curves for 1 (black), 2 (blue), 3 (red), 4 (olive), 5 (magenta) and 6 (purple).