Supplementary Material (ESI) for Chemical Communications

A novel 3D porous metal–organic framework based on trinuclear cadmium clusters as a promising luminescent material exhibiting tunable emissions between UV and visible wavelengths

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Syntheses: 2,6-di-(4-triazolyl)pyridine (**L**) ligand was synthesized using the literature method.[S1] Compound **1**: **L** (92.4 mg, 0.4 mmol) and $Cd(BF_4)_2 \cdot 6H_2O$ (78.8 mg, 0.2 mmol) were heated under reflux in H_2O for 2h and then the resulting solution was filtered. Colorless single-crystals suitable for X-ray diffraction were obtained by slow evaporation in glass vial within several days. Yield: 48%. IR (KBr): *m* = 3446.3m, 3108.2s, 2360.5m, 1611.3s, 1532.5vs, 1465.2vs, 1398.2w, 1283.3s, 1253.2m, 1097.0w, 1060.6s, 891.2m, 807.3s, 770.8s, 750.2s, 628.9s, 469.4m cm^{-1}. Anal. (%): found (calc.): $C_{54}H_{71}B_2Cd_3F_{14}N_{42}O_{15.50}Si$, C: 30.54 (29.36), H: 3.25 (3.24), N: 26.53 (26.63).

X-ray Crystallography: Crystal data was collected on Bruker SMART 1000 CCD detector with graphite-monochromated Mo-Kα radiation (λ = 0.71073 Å) at 294(2) K. compound **1**, $C_{54}H_{71}B_2Cd_3F_{14}N_{42}O_{15.5}Si$, M = 2209.44, Rhombohedral, R-3, a = 20.1077(11), b = 20.1077(11), c = 20.234(2) Å, α = 90°, β = 90°, γ = 120°, V=7085.1(9) $Å^3$, Z = 3, μ = 0.787 mm^{-1}, Dc = 1.553 Mg m^{-3}, F(000) = 3321, R_{int} = 0.0317, 13502 reflections, 3224 with I > 2σ (I) for 252 parameters, R_1 = 0.0413 for I > 2σ (I), R_1 = 0.0495 and wR_2 = 0.1357 for all data, G_OF = 1.009. The structures were solved by direct methods and refined with the full-matrix least-squares technique using the SHELXS-97 [S2]and SHELXL-97 programs. [S3]

CCDC 614743. For crystallographic data in CIF or other electronic format see DOI: 10.1039/b000000x

Characterization: Elemental analysis for C, H and N were carried out with a Perkin-Elmer 240 elemental analyzer. The FT-IR spectra were measured with a Bruker Tensor 27 Spectrometer on KBr disks. The fluorescent spectrum was measured on a Varian Cary Eclipse Fluorescence spectrophotometer. Powder X-ray diffraction measurements were recorded on a D/Max-2500 X-ray diffractometer using Cu-Kα radiation. Thermal analyses (under an nitrogen atmosphere, heating rate of 5 ℃ min^{-1}) were carried out in a Labsys NETZSCH TG 209 Setaram apparatus.

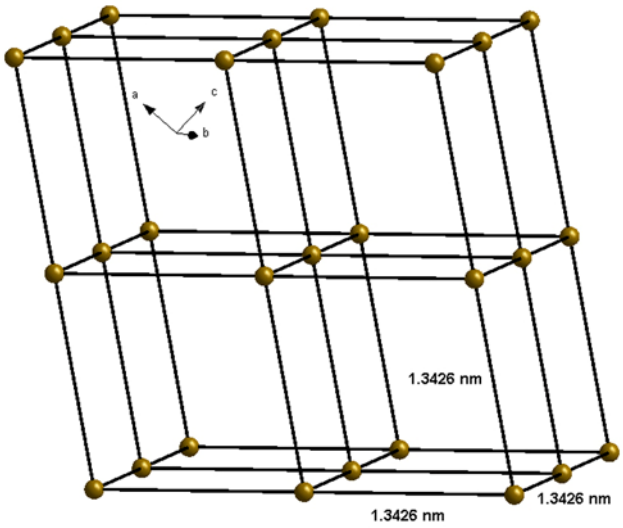

Figure S1. Topological representation of compound **1** showing a rhombohedral coordination network. The $[Cd_3L_{12}]$ trinuclear clusters are taken as nodes of the framework.

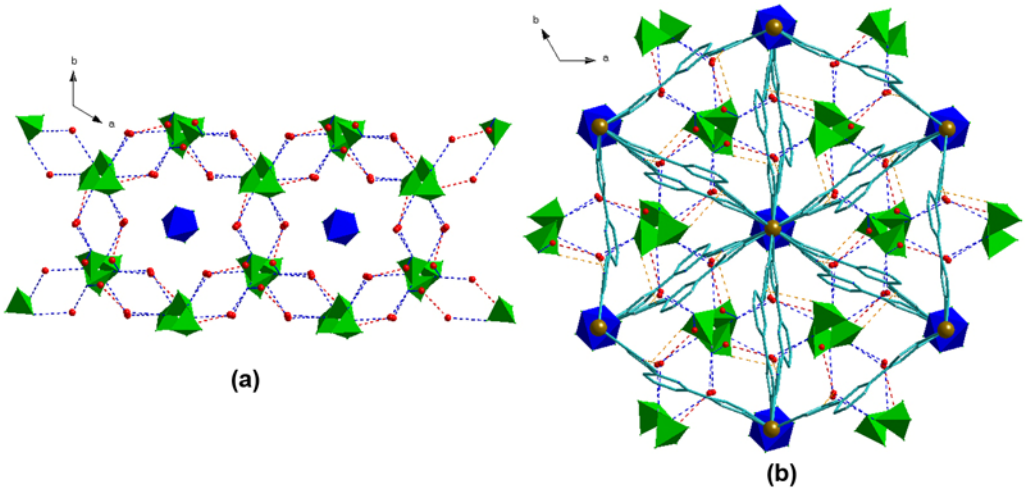

Figure S2. (a) Hydrogen-bonded interactions of the water molecules and anions without the framework. (b) A perspective view showing the interactions of the water molecules and anions with the MOF along the *c* axis. Color code: Cd, brown; O, red; SiF_6^{2-}, polyhedron, blue; BF_4^-, polyhedron, green.

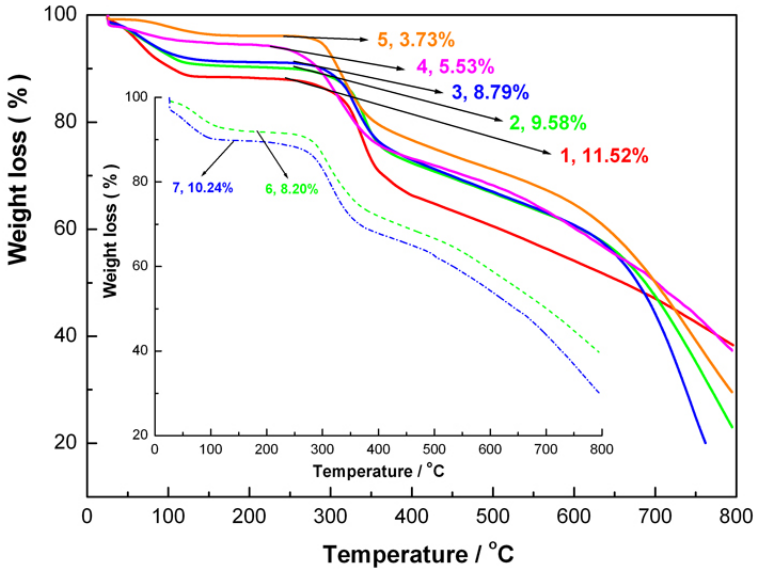

Figure S3. TGA curves of complex **1-5**. Color lines: **1**, red; **2**, green; **3**, blue; **4**, magenta; **5**, orange. The inset pictures represent the TGA curves of complex **6** and **7**. Color scheme: **6**, dash line, green; **7**, dash-dot line, blue.

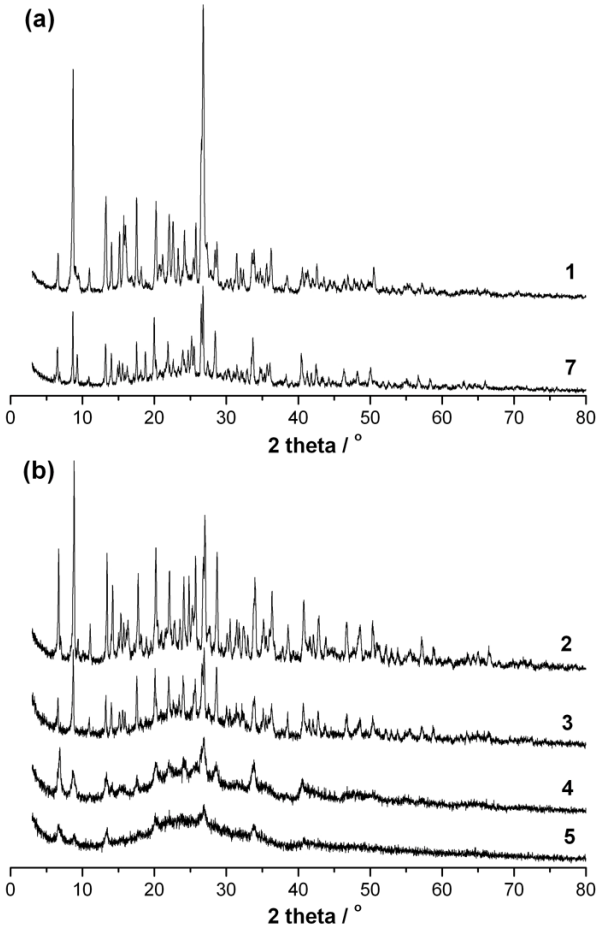

Figure S4. PXRD patterns of (a) a fresh sample **1** and rehydration sample **7**, (b) complexes **2-5**, after heat treatment of sample **1**.

References

S1 H. W. Richard and J. H. Albert, *J. Org. Chem.*, **1953**, *18*, 1368.

S2 G.M. Sheldrick, SHELXS-97, Program for X-ray Crystal Structure Solution, Göttingen University, Germany, **1997**.

S3 G.M. Sheldrick, SHELXL-97, Program for X-ray Crystal Structure Refinement, Göttingen University, Germany, **1997**.