Electronic Supplementary Information (ESI)

An unprecedented organic-inorganic hybrid material with the I^{3}O^3 framework based on cadmium hydroxide and in situ generated 1H-tetrazolate-5-acetic acid

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Materials and instruments

All chemicals were commercially available sources of analytical grade and used without further purification. The elemental analyses were performed on an Elementar Vario EL III microanalyzer. The FT-IR spectra were obtained on a Perkin-Elmer Spectrum using KBr disks in the range 4000–400 cm^{-1}. Photoluminescent analysis was performed on an Edinburgh EI920 fluorescence spectrometer with a 450-W Xe lamp and a R928P PMT detector. A 399-nm high-pass filter was applied when performing PL determinations. Thermogravimetric analysis (TGA) experiment was made on a METTLER TOLEDO TGA/DSC1 thermogravimetric analyzer under N_2 atmosphere with the sample heated in an Al_2O_3 crucible at a heating rate of 10 K min^{-1}. Powder X-ray diffraction (PXRD) data were collected on a Miniflex II diffractometer using Cu-$K\alpha$ radiation (λ = 1.540598 Å) at 40 kV and 40 mA in the range of $5° \leq 2\theta \leq 60°$. The simulated patterns were derived from the Mercury Version 1.4 software (*http://www.ccdc.cam.ac.uk/products/mercury/*). Single crystal X-ray diffraction was carried out by a Rigaku Mercury CCD diffractometer using graphite monochromated with Mo-K_α radiation (λ = 0.71073 Å). There was no evidence of crystal decay during data collection. The intensity data sets were collected with the ω scan technique and corrected for Lp effects. The SHG measurement on hand-selected unsieved crystalline sample of **1** was performed on a modified Kurtz-NLO system using 1.06 and 1.94 um laser radiation, respectively. The SHG signal was collected in a reflection geometry from the excitation surface and focused into a fiber optic bundle. The output of the fiber optic bundle was coupled to the entrance slit of a spectrometer and detected using a CCD detector. Potassium dihydrogen phosphate (KDP) powder was used as a reference to assume the second-order NLO effect. No obvious SHG signals were detected when irradiated by 1.94 um/1.06 um laser.

Table S1 The selected bond distances for **1**^{a}.

Cd(1)-O(3)#1	2.247(2)	Cd(2)-O(3)	2.256(3)
Cd(1)-O(3)	2.247(2)	Cd(2)-O(3)#4	2.301(2)
Cd(1)-O(1)#2	2.347(3)	Cd(2)-N(3)#5	2.313(3)
Cd(1)-O(1)#3	2.347(3)	Cd(2)-N(1)#6	2.362(3)
Cd(1)-N(4)#1	2.358(3)	Cd(2)-O(1)#3	2.455(2)
Cd(1)-N(4)	2.358(3)	Cd(2)-O(2)#6	2.498(2)

[a] Symmetry codes for **1**: (#1) –x, –y + 1, z; (#2) –x + 1/2, –y + 1, z + 1/2; (#3) x – 1/2, y, z+ 1/2; (#4) x – 1/4, –y + 3/4, z + 1/4; (#5) –x – 1/4, y – 1/4, z + 1/4; (#6) –x, –y + 1, z + 1.

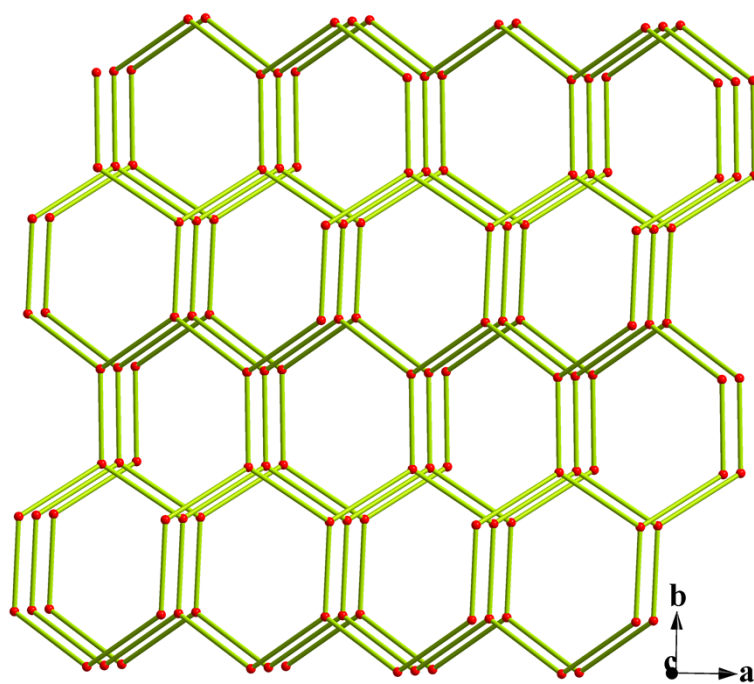**Fig. S1** The 3-D inorganic ths (ThSi$_2$) top network.

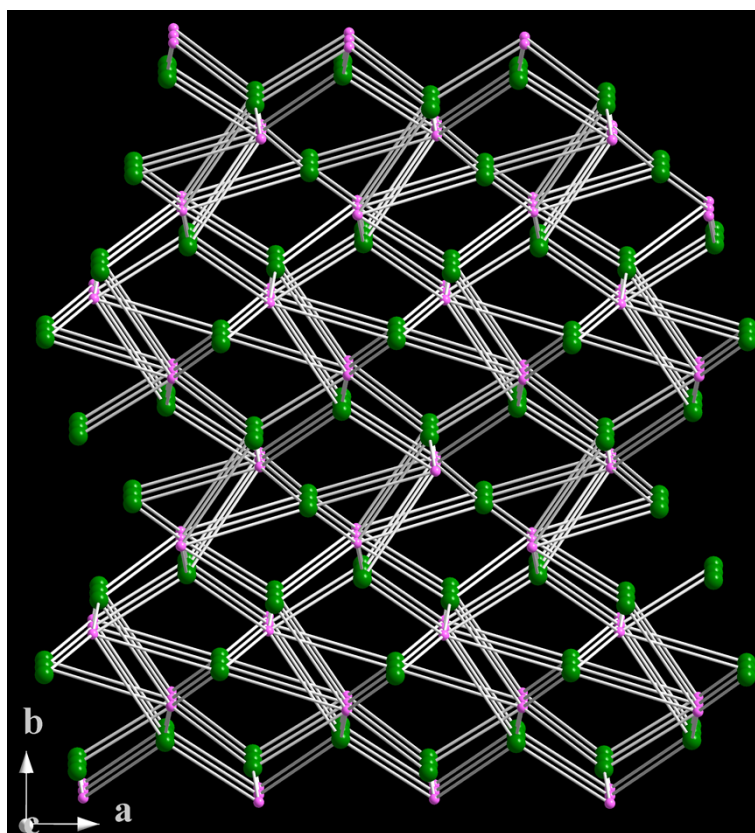**Fig. S2** The 3-D organic (4,4,6)-connected topology. Green: Cd(II), pink: tza^{2-}.

Fig. S3 (a) The simplified (3,6,6,6-*c*) topological net of **1**; (b, c) View of a right-handed helical chain along with the appearance of μ_6-tza^{2-} ligands from the *c*-axis and *b*-axis, respectively (the atoms in red, pink and green represent the μ_3-OH$^-$, μ_6-tza^{2-} and Cd(II), respectively).
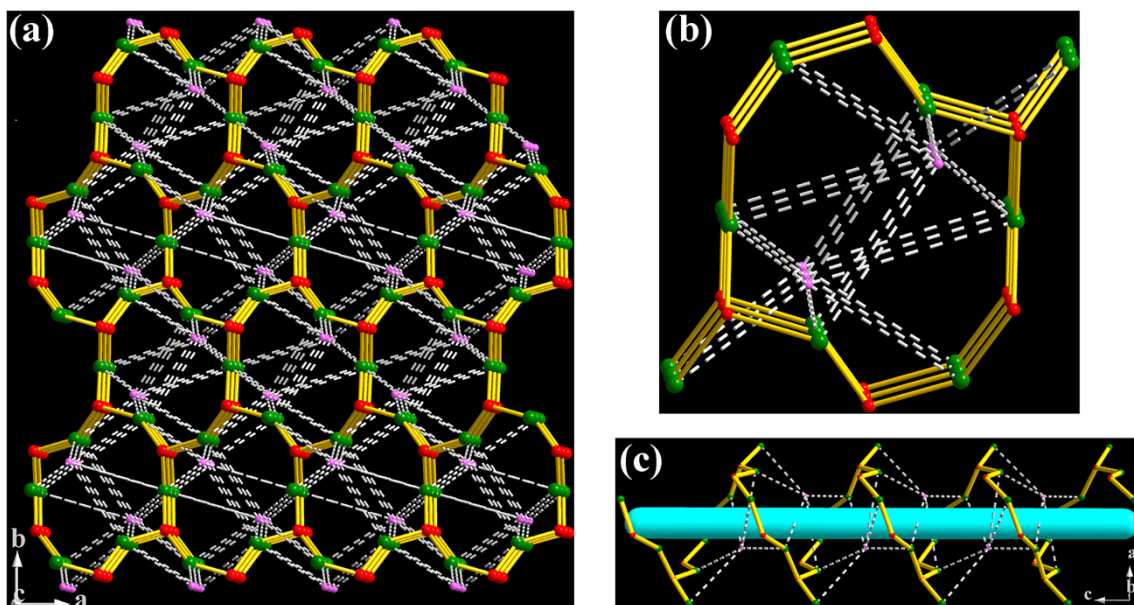

Fig. S4 Powdered X-ray diffraction (PXRD) patterns of **1**. The black and blue lines represent simulated and experimental results, respectively.
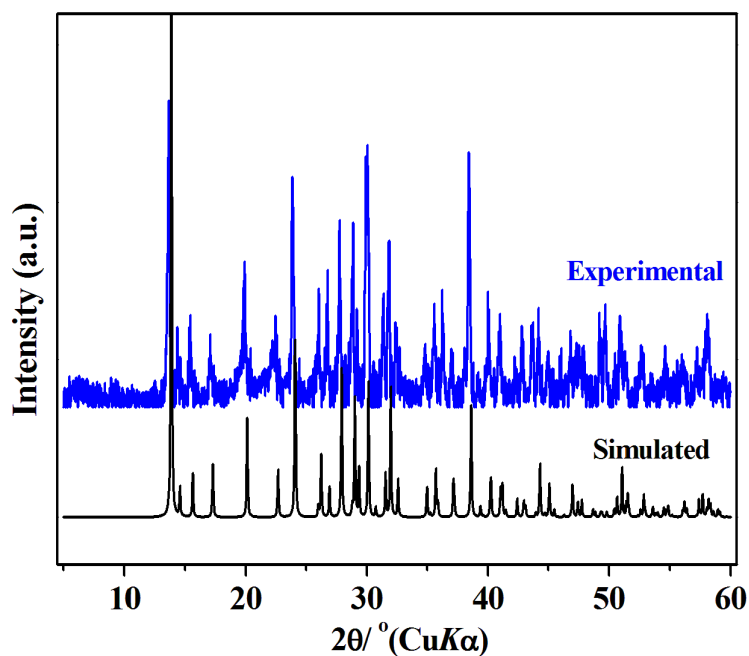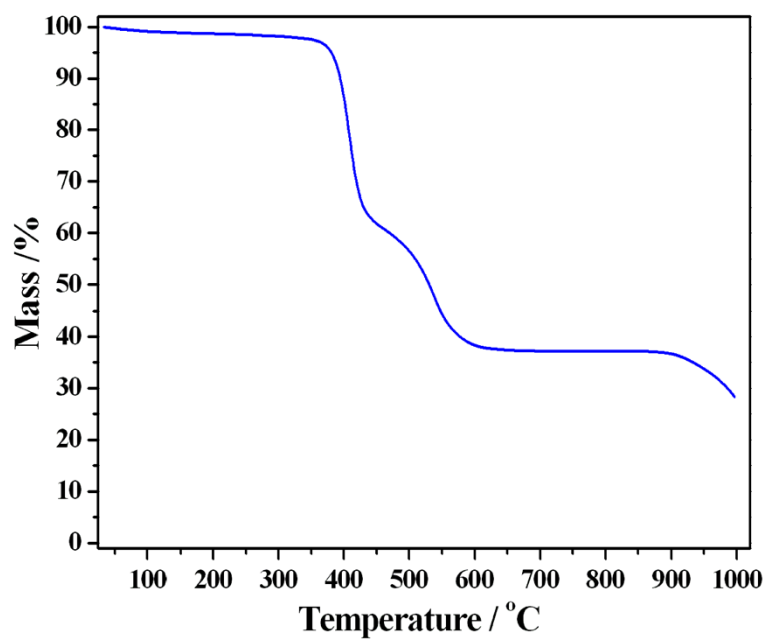
Fig. S5 View of the TGA curve of **1**.

Fig. S6 The FT-IR spectra of **1**.