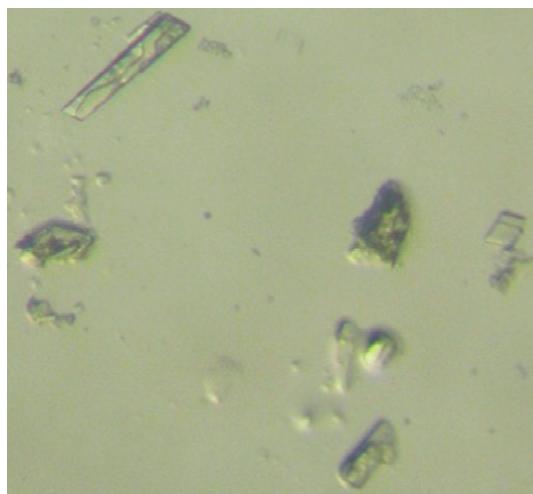


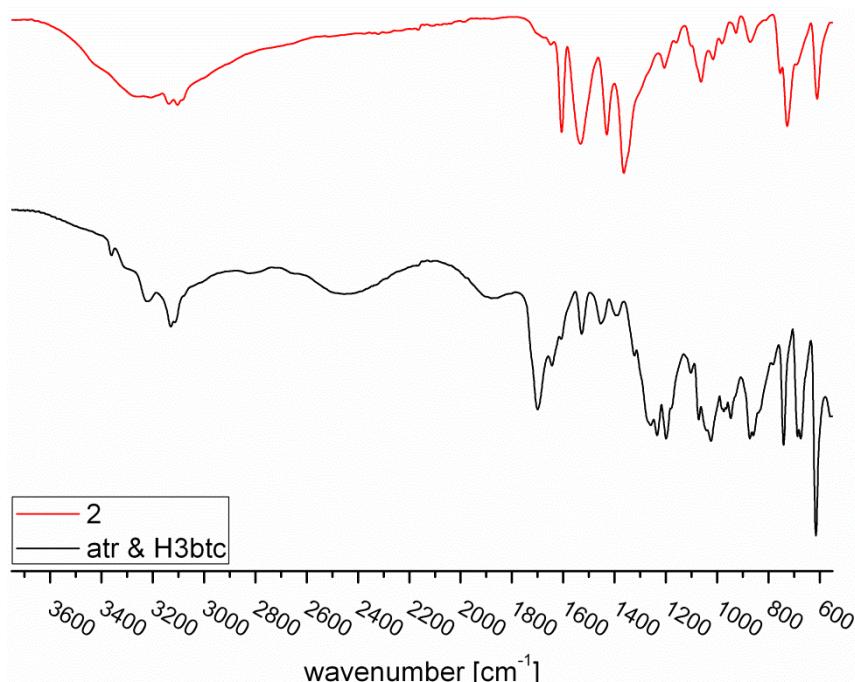
Supporting Information

## Supplementary Materials: A Cadmium Anionic 1-D Coordination Polymer $\{[\text{Cd}(\text{H}_2\text{O})_6][\text{Cd}_2(\text{atr})_2(\mu_2\text{-btc})_2(\text{H}_2\text{O})_4]\ 2\text{H}_2\text{O}\}_n$ within a 3-D Supramolecular Charge-Assisted Hydrogen-Bonded and $\pi$ -Stacking Network

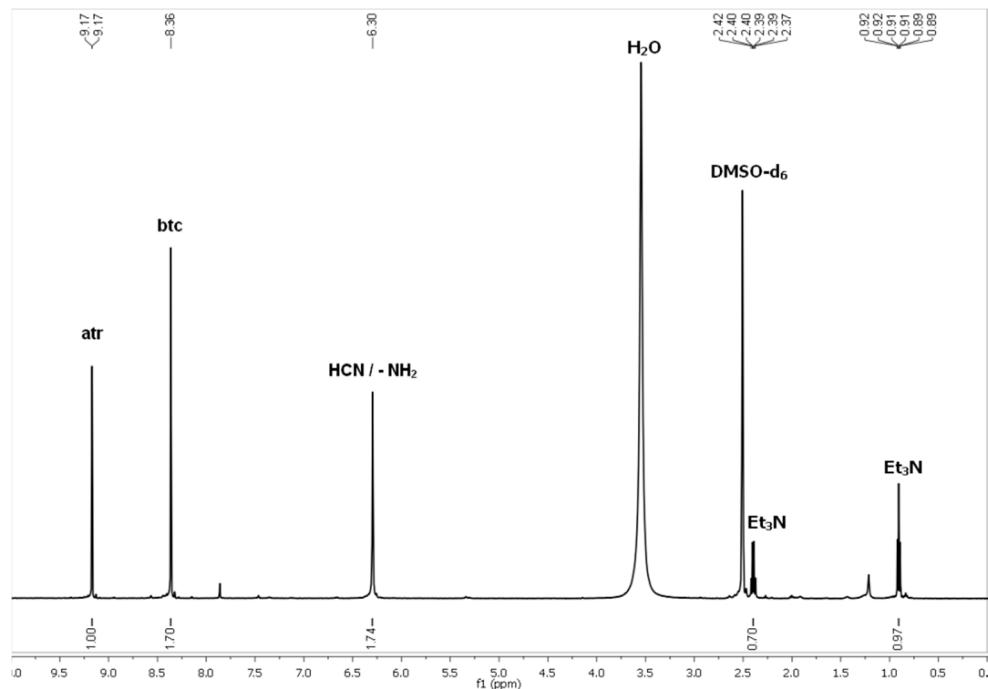
Anas Tahli, Ümit Köc, Reda F. M. Elshaarawy, Anna Christin Kautz, Christoph Janiak



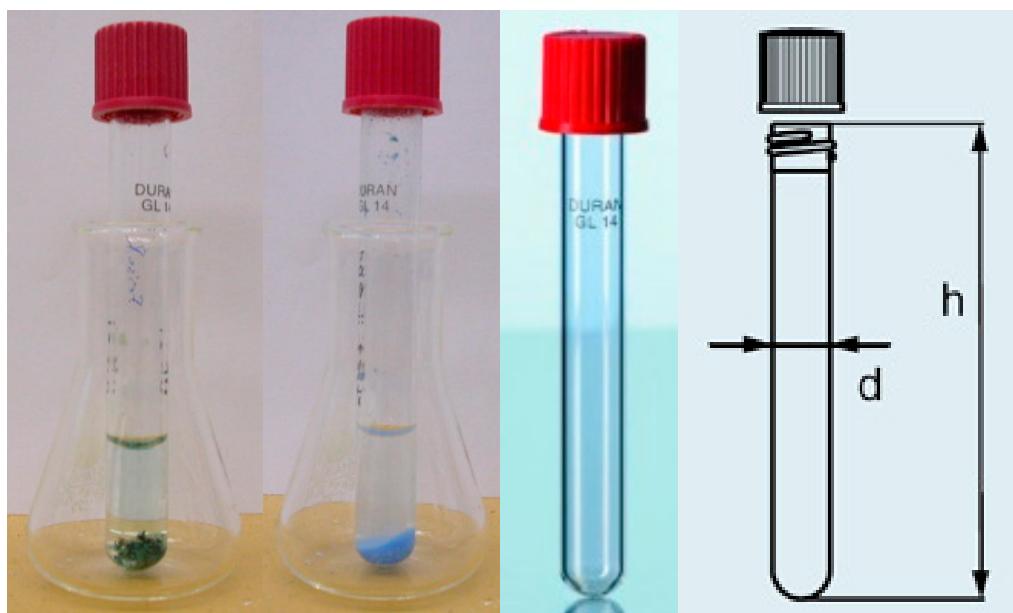
**Figure S1.** Colorless crystals of 1-D  $\{[\text{Cd}(\text{H}_2\text{O})_6][\text{Cd}_2(\text{atr})_2(\mu_2\text{-btc})_2(\text{H}_2\text{O})_4]\ 2\text{H}_2\text{O}\}_n$  **1**.



**Figure S2.** IR spectra (ATR) for comparison between the compound **1** and mixed ligands of atr and H<sub>3</sub>btc.



**Figure S3.**  $^1\text{H}$  NMR Spectrum (500 MHz) of **1** in  $\text{DMSO-d}_6$  after addition of an excess of  $\text{NaCN}$  to the solution.

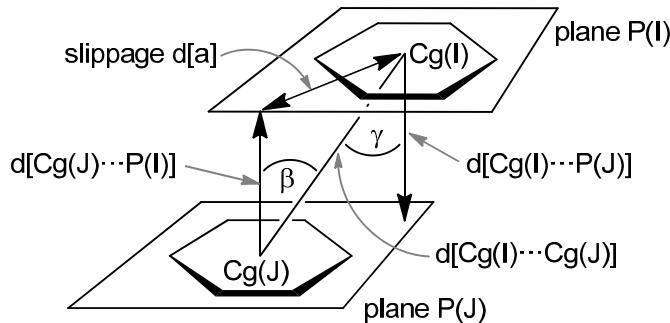


**Figure S4.** Used DURAN® culture glass tube for coordination polymer synthesis up to 150 °C instead of autoclave to obtain single crystals suitable for X-ray diffraction measurements.

#### Analysis of Supramolecular $\pi$ -Stacking Interactions in the Structure of **1**.

Packing Analysis by PLATON [1,2].

The listed "Analysis of Short Ring-Interactions" in the PLATON geometry calculation for possible  $\pi$ -stacking interactions yielded rather short centroid-centroid contacts ( $<3.8 \text{ \AA}$ ), near parallel ring planes ( $\alpha < 10^\circ$  to  $\sim 0^\circ$  or even exactly  $0^\circ$  by symmetry), small slip angles ( $\beta, \gamma < 25^\circ$ ), and vertical displacements (slippage  $< 1.5 \text{ \AA}$ ) which translate into a sizable overlap of the aryl-plane areas [3–10].



**Scheme S1.** Graphical presentation of the parameters used for the description of  $\pi$ - $\pi$  stacking interactions.

Packing analysis for possible  $\pi$ - $\pi$  interactions in **1** (see Scheme S1 for explanation):

=====

Analysis of Short Ring-Interactions with Cg-Cg Distances < 6.0 Å and Beta,  $\beta$  < 60.0°.

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- Cg(I) = Plane number I (= ring number in ( ) above)
- $\alpha$  = Dihedral Angle between Planes I and J (°)
- $\beta$  = Angle Cg(I)-->Cg(J) vector and normal to plane I (°)
- $\gamma$  = Angle Cg(I)-->Cg(J) vector and normal to plane J (°)
- $d[Cg(I)\dots Cg(J)]$  = Distance between ring Centroids (Å)
- $d[Cg(I)\dots P(J)]$  = Perpendicular distance of Cg(I) on ring J (Å)
- $d[Cg(J)\dots P(I)]$  = Perpendicular distance of Cg(J) on ring I (Å)
- Slippage  $d[a]$  = Distance between Cg(I) and Perpendicular Projection of Cg(J) on Ring I (Å).

**Table S1.** Packing analysis for possible  $\pi$ - $\pi$  interactions in **1**

| Cg(I) | Cg(J) | [ARU(J)]  | $d[Cg-Cg]$<br>(Å) | $\alpha$<br>(°) | $\beta$<br>(°) | $\gamma$<br>(°) | $d[Cg(I)\dots P(J)]$<br>(Å) | $d[Cg(I)\dots P(J)]$<br>(Å) | Slippage<br>$d[a]$ (Å) |
|-------|-------|-----------|-------------------|-----------------|----------------|-----------------|-----------------------------|-----------------------------|------------------------|
| Cg(1) | Cg(1) | [3766.01] | 3.997(4)          | 0               | 27.99          | 27.99           | 3.529(3)                    | -3.530(3)                   | 1.876                  |
| Cg(1) | Cg(1) | [3767.01] | 3.598(4)          | 0               | 26.41          | 26.41           | 3.529(3)                    | 3.222(3)                    | 1.600                  |
| Cg(1) | Cg(2) | [4554.01] | 3.726(4)          | 4               | 20.33          | 23.85           | 3.408(3)                    | -3.494(3)                   | -                      |
| Cg(1) | Cg(2) | [4555.01] | 3.726(4)          | 4               | 23.85          | 20.33           | -3.494(3)                   | 3.408(3)                    | -                      |

[3766] = 2 - X, 1 - Y, 1 - Z; [3767] = 2 - X, 1 - Y, 2 - Z; [4554] = X,  $\frac{1}{2}$  - Y, -1/2 + Z; [4555] = X, 1/2 - Y, 1/2 + Z; The Cg(I) refer to the ring center-of-gravity numbers given in; Cg(1) = Ring N1-N2-C10-N3-C11; Cg(2) = Ring C2-C3-C4-C5-C6-C7.

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