

Supplementary Materials:

Reactions of Cadmium(II) Halides and Di-2-pyridyl Ketone Oxime: One-dimensional Coordination Polymers

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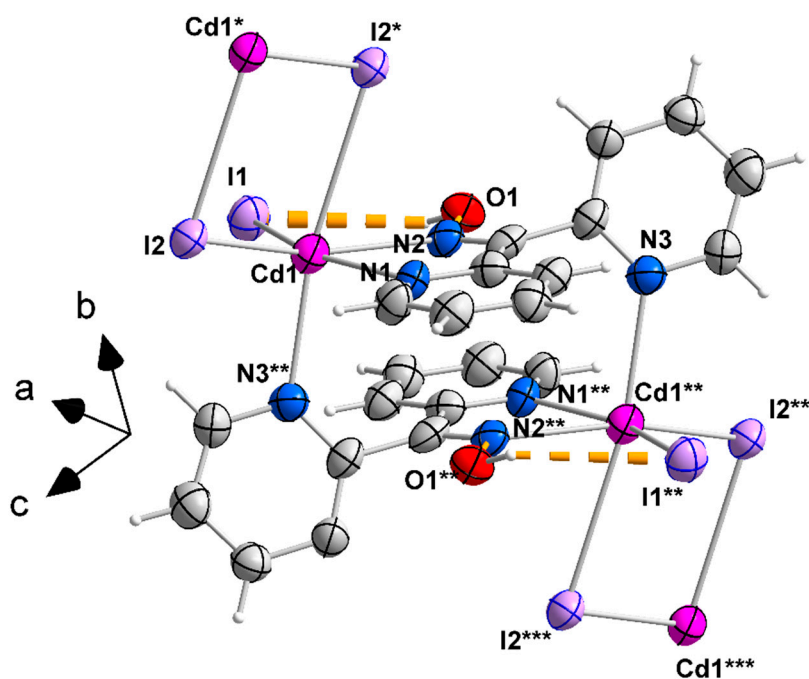


Figure S1. Complete coordination spheres of two neighboring Cd^{II} centers (Cd1, Cd1**) in one zigzag chain of complex 3. The symmetry codes are the same with those mentioned for compound 2 in Figure 2b.

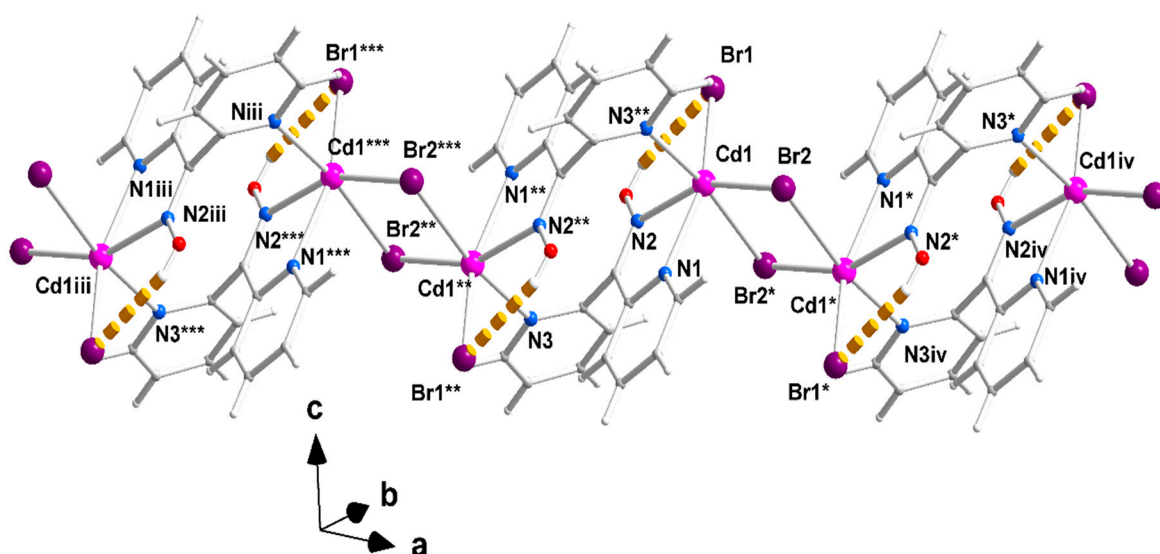


Figure S2. A portion of one zigzag chain (developed along the [1, 1, 0] crystallographic direction) of complex **2**. The thick dashed orange lines represent intrachain $O_{\text{oxime}}\text{-H}\cdots\text{Br}_{\text{terminal}}$ H bonds. The symmetry codes (*), (**) and (***) are the same with those described in Figure 2b, and the additional codes are: (iii) $0.5-x, 0.5-y, 1-z$ and (iv) $0.5+x, 0.5+y, z$.

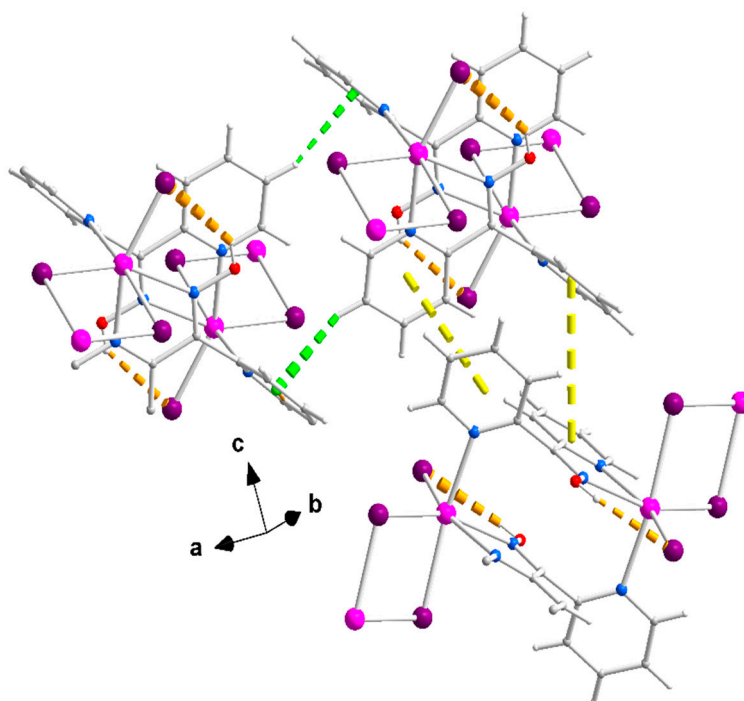


Figure S3. Interactions between neighboring chains in the crystal structure of compound **2**. The thick dashed light green and yellow lines indicate $\text{C2-H2}\cdots\text{Cg1}$ ($\text{C-H}\cdots\pi$) and π - π interactions, respectively; for details, see text. The thick dashed orange lines represent intrachain $O_{\text{oxime}}\text{-H}\cdots\text{Br}_{\text{terminal}}$ H bonds (also see Figures 2b and 4).

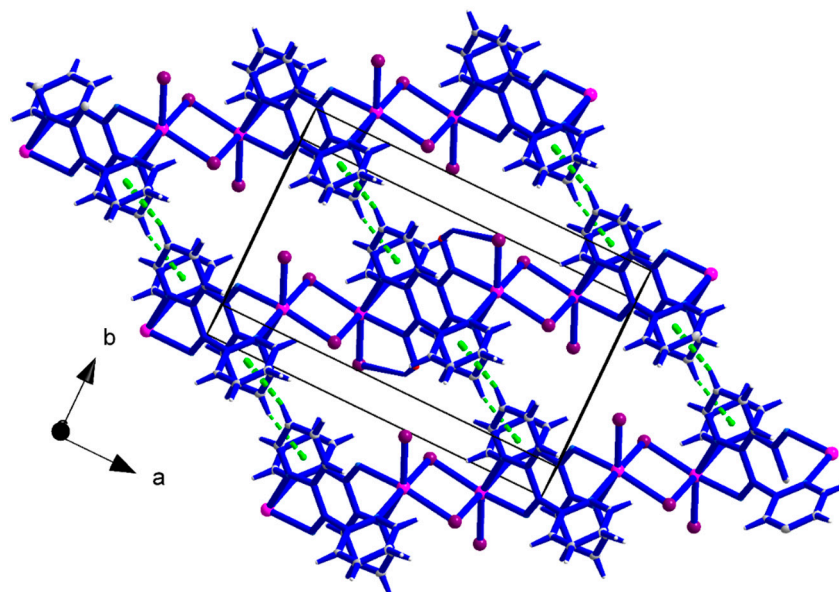
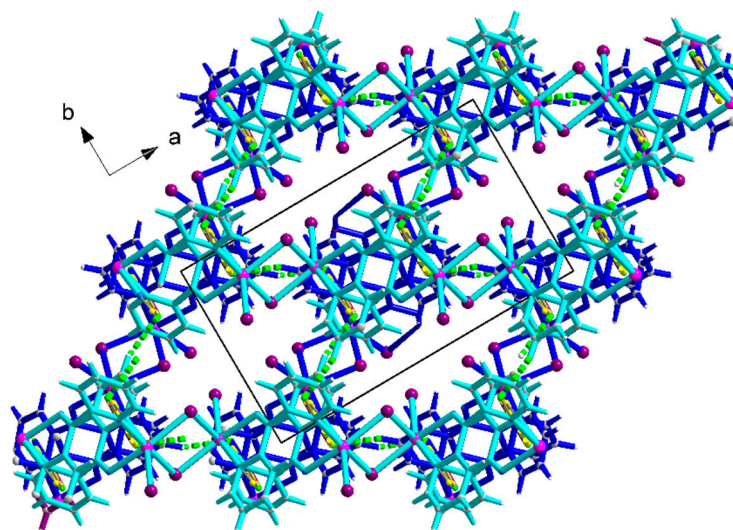
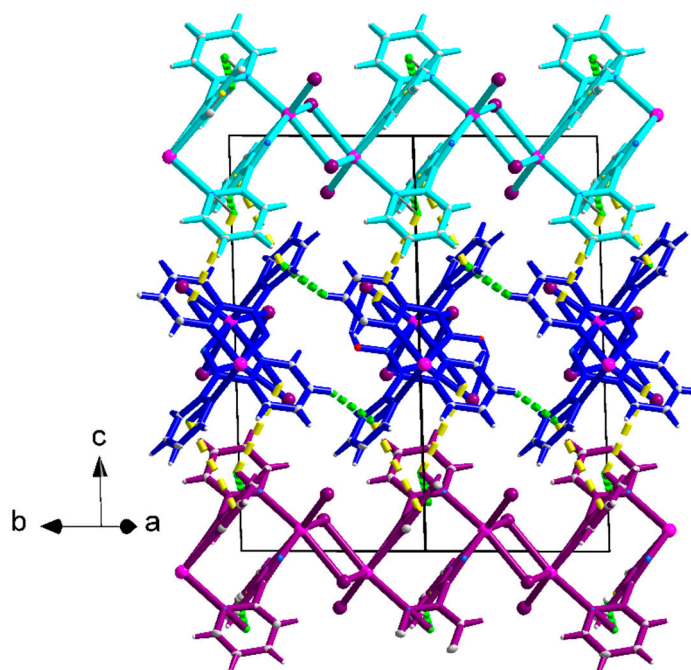


Figure S4. Layers of chains parallel to the (001) crystallographic planes in the structures of **2** and **3**. The chains are represented by thick blue solid lines and the C2-H2...Cg1 (C-H... π) interactions are indicated with thick dashed light green lines; for details, see text.



(a)



(b)

Figure S5. (a) Neighboring layers of **2** and **3** stacked along the c axis with a crossed-arrangement fashion relative to each other; in the top layer (cyan solid lines), the chains extend along the $[-1, 1, 0]$ direction and in the bottom one (blue solid lines) along $[1, 1, 0]$. (b) Alternate stacking in **2** and **3** along the c axis; at the bottom (violet solid lines) and top (cyan solid lines) layers, the chains are along $[-1, 1, 0]$ and in the middle one (blue solid lines) are along $[1, 1, 0]$. The thick dashed yellow and light green lines indicate $C-H\cdots\pi$ and $\pi-\pi$ interactions; see also caption of Figure S2.

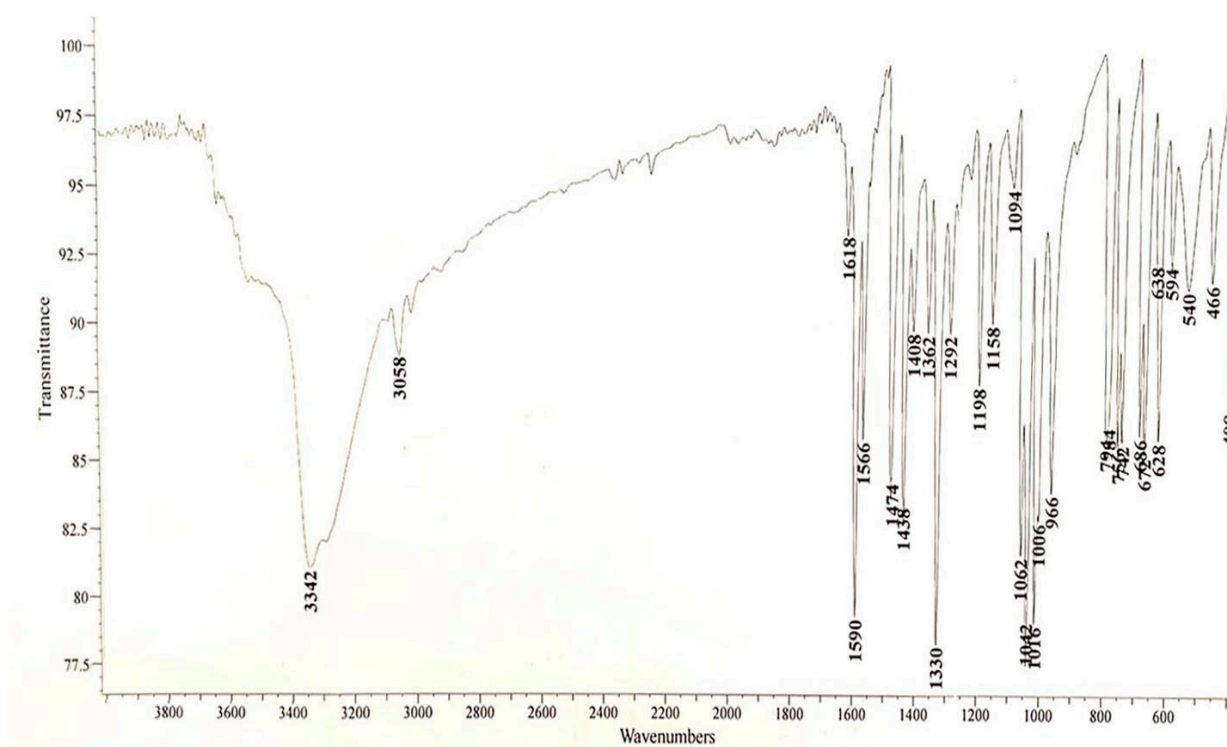


Figure S6. The IR spectrum (KBr, cm^{-1}) of the 1D polymer 2.

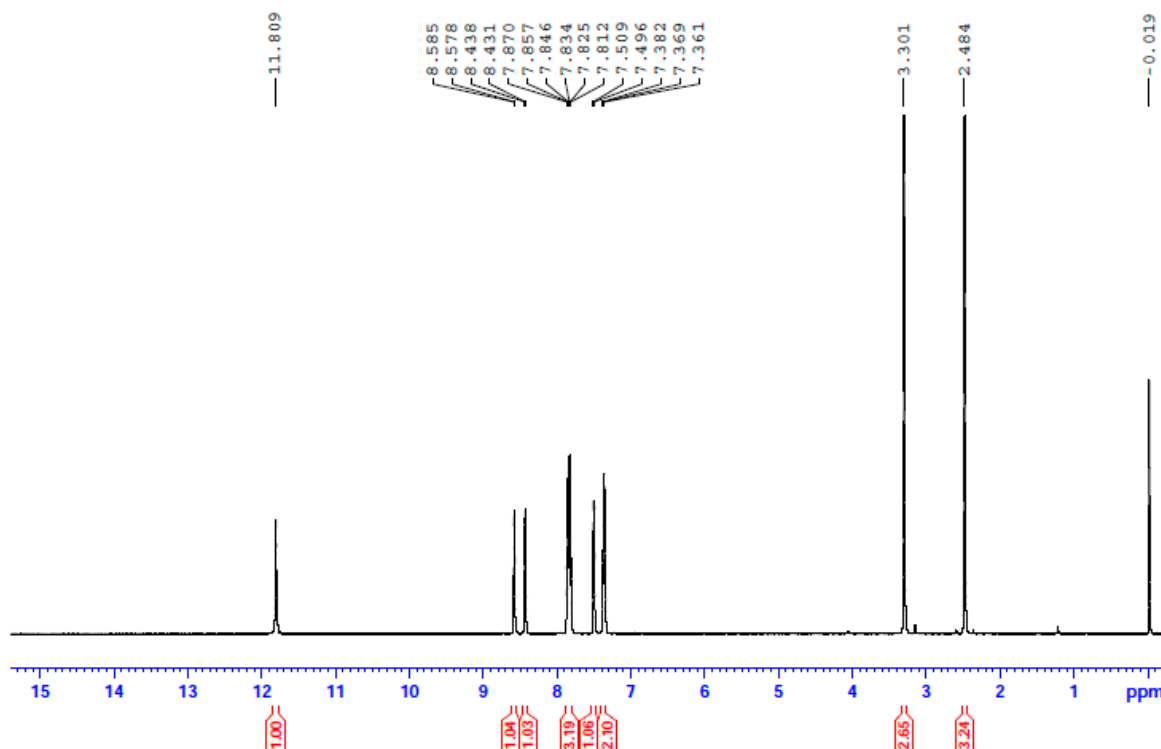


Figure S7. The ^1H NMR spectrum of $1 \cdot 2\text{H}_2\text{O}$ in $\text{d}_6\text{-DMSO}$. The signal at δ 2.48 ppm is due to the methyl groups of the non-deuteriated amount of the solvent, and the signal at δ 3.30 ppm to the protons of the lattice H_2O and the water content of the solvent.

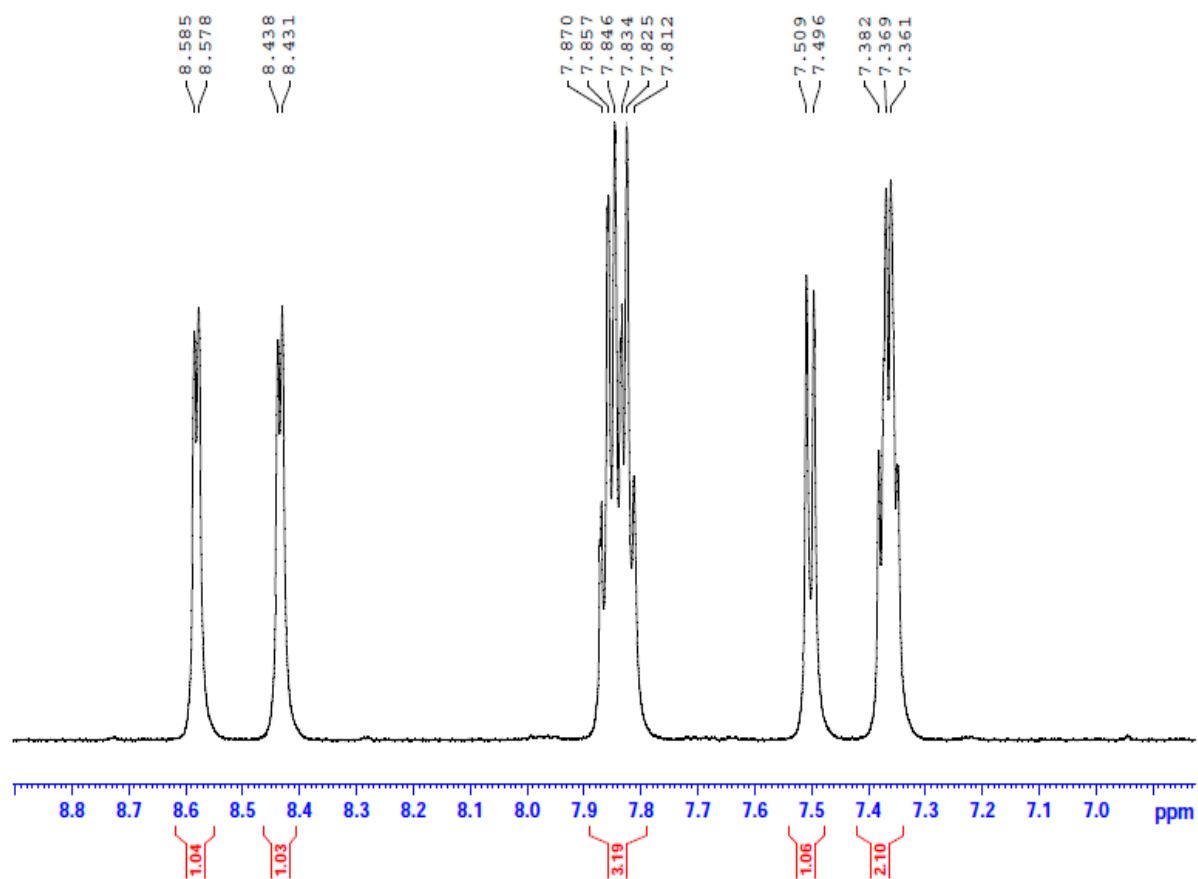


Figure S8. The ^1H NMR spectrum of 2 in d_6 -DMSO in the aromatic region.