

Electronic Supplementary Material (ESI) for RSC Advances.
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Electronic Supporting Information

Cadmium(II) complexes of *N,N'*-dimethyl violuric acid containing benzimidazole and pyridine as ancillary ligands : Synthesis, characterization, crystal structures and DFT study

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1. Figures S1–S2

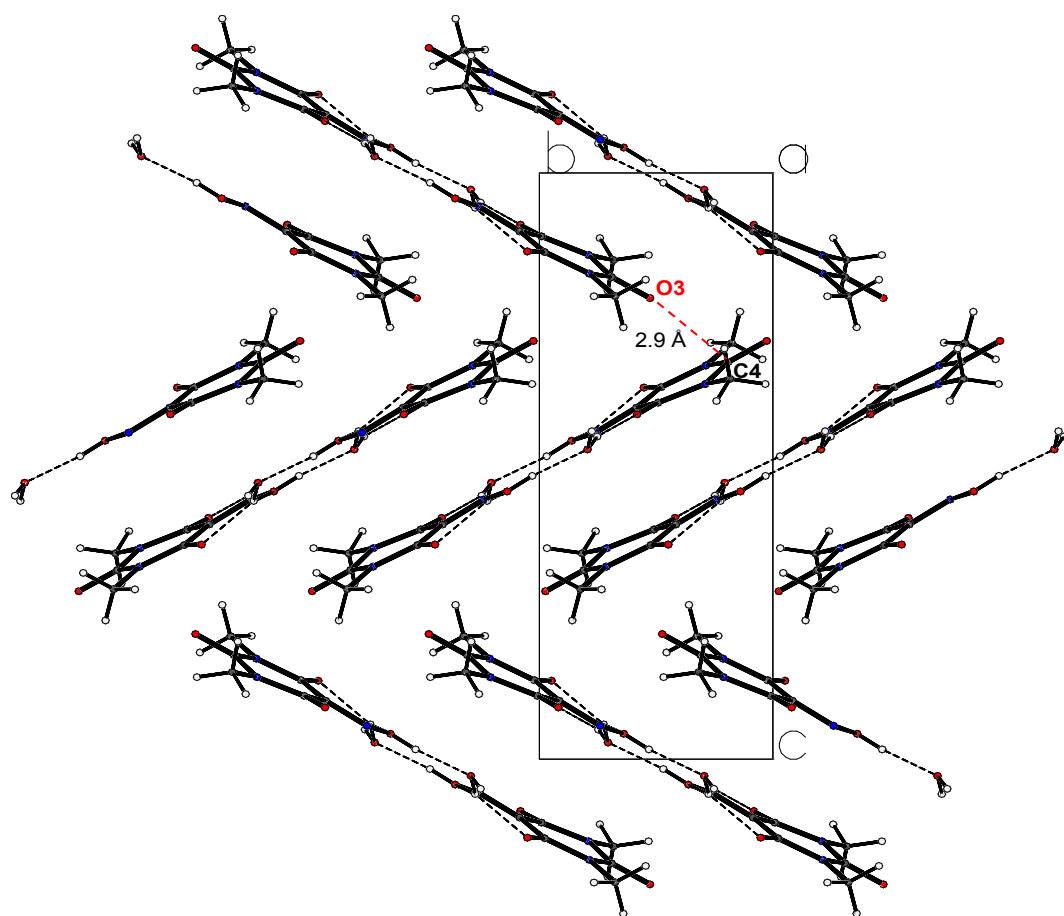


Fig.S1 1-D chains of $\{1(\mu\text{-H}_2\text{O})\}_2$ along a and stacked tilted along b

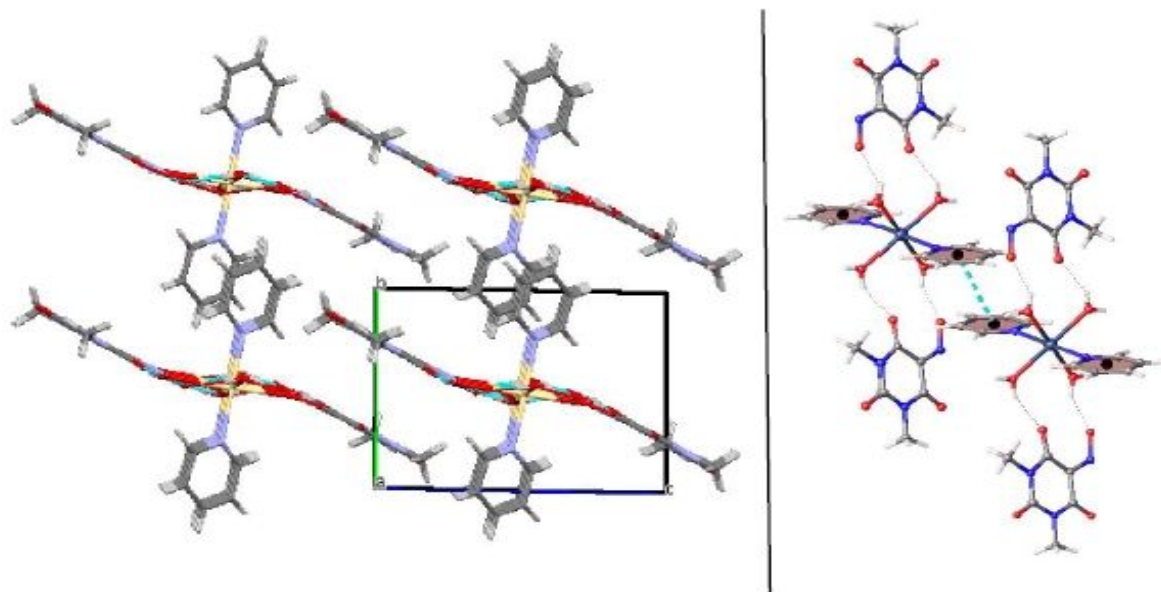


Fig. S2 Left: Packing of the one-dimensional chains in **3**. Right: π -stacking between the pyridine rings (ring-ring-distance 3.6 Å) in **3**.

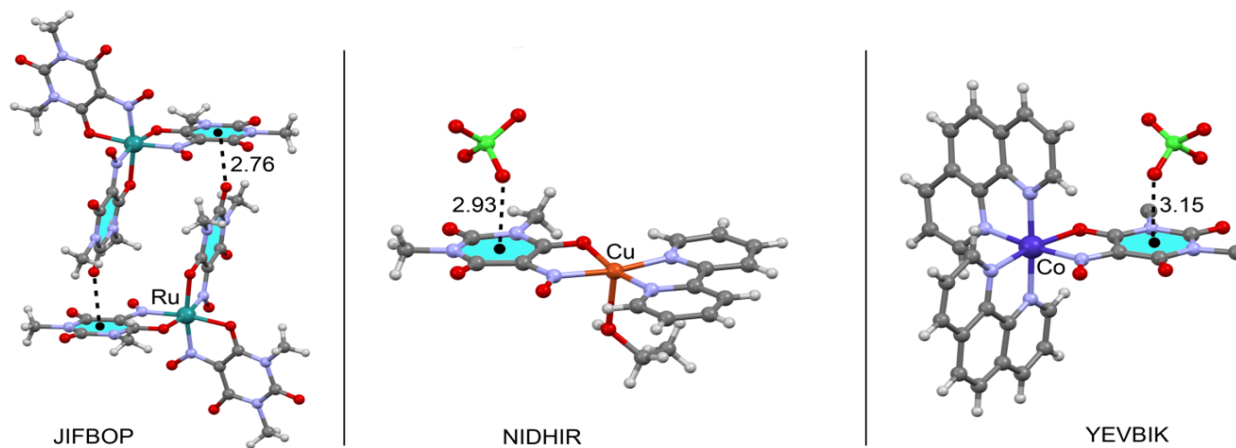


Fig. S3 Partial views of several X-ray structures retrieved from the CSD. Distances in Å. CSD reference codes are indicated.

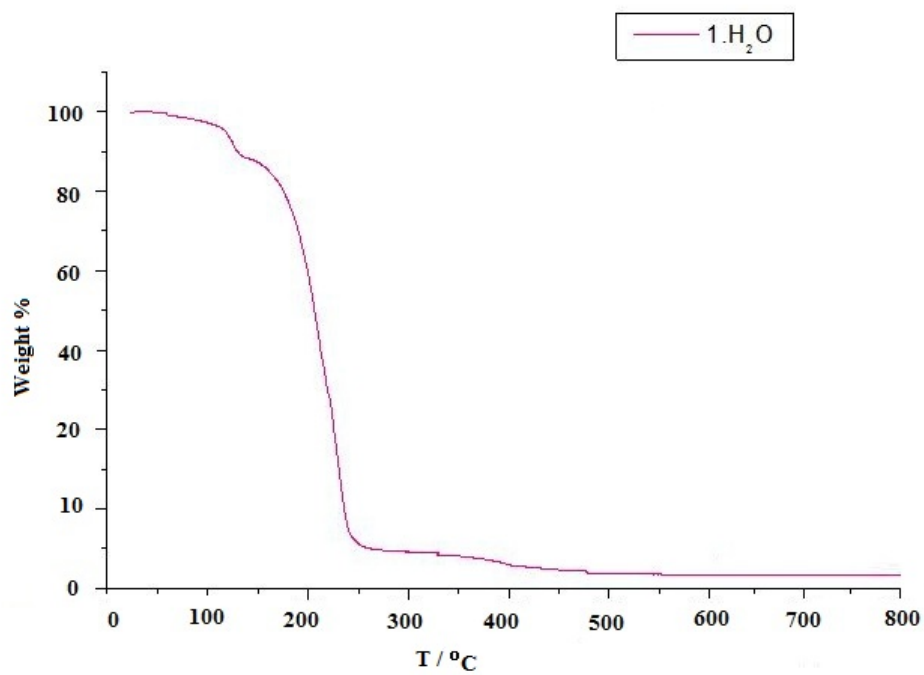


Fig. S4 TGA of HDMV (1·H₂O)

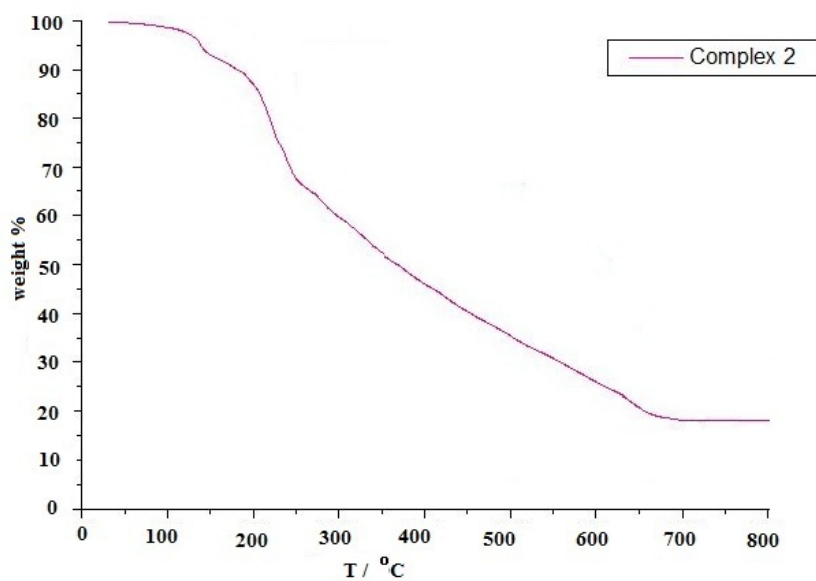


Fig. S5 TGA of [Cd(DMV)₂(Benzim)₂] (2)

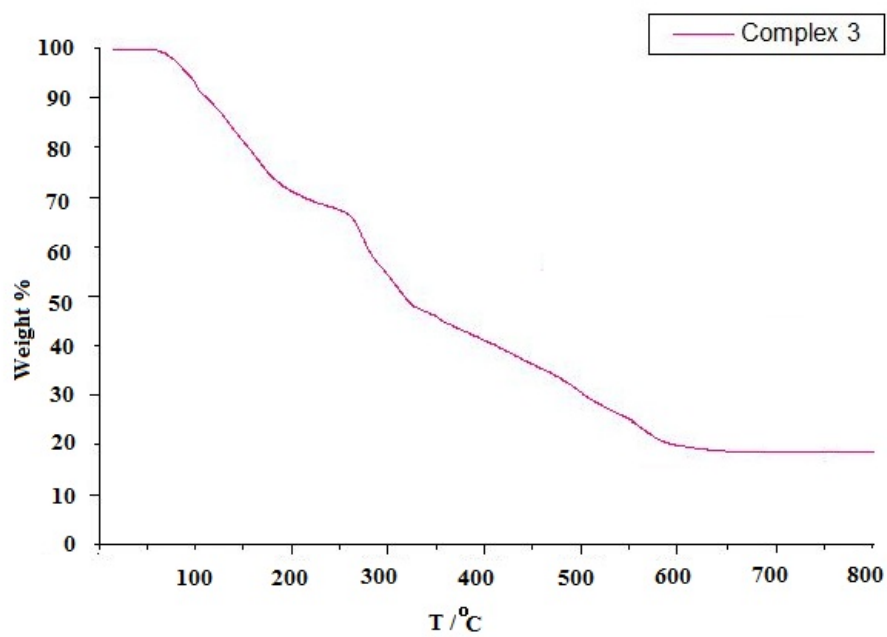


Fig. S6 TGA of $[\text{Cd}(\text{H}_2\text{O})_4(\text{py})_2](\text{DMV})_2$ (**3**)

2. IR and NMR spectra:

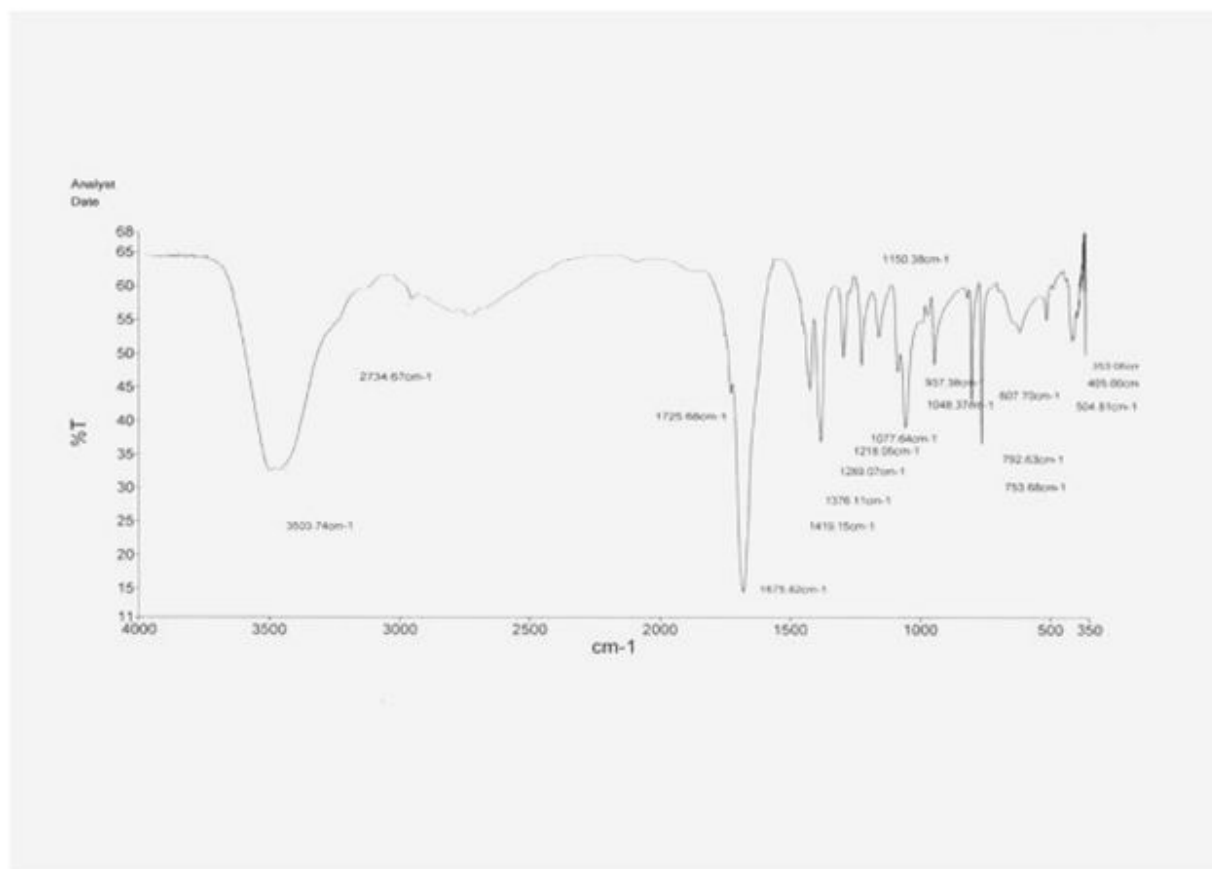


Fig.S7 IR Spectrum of HDMV (1-H₂O)

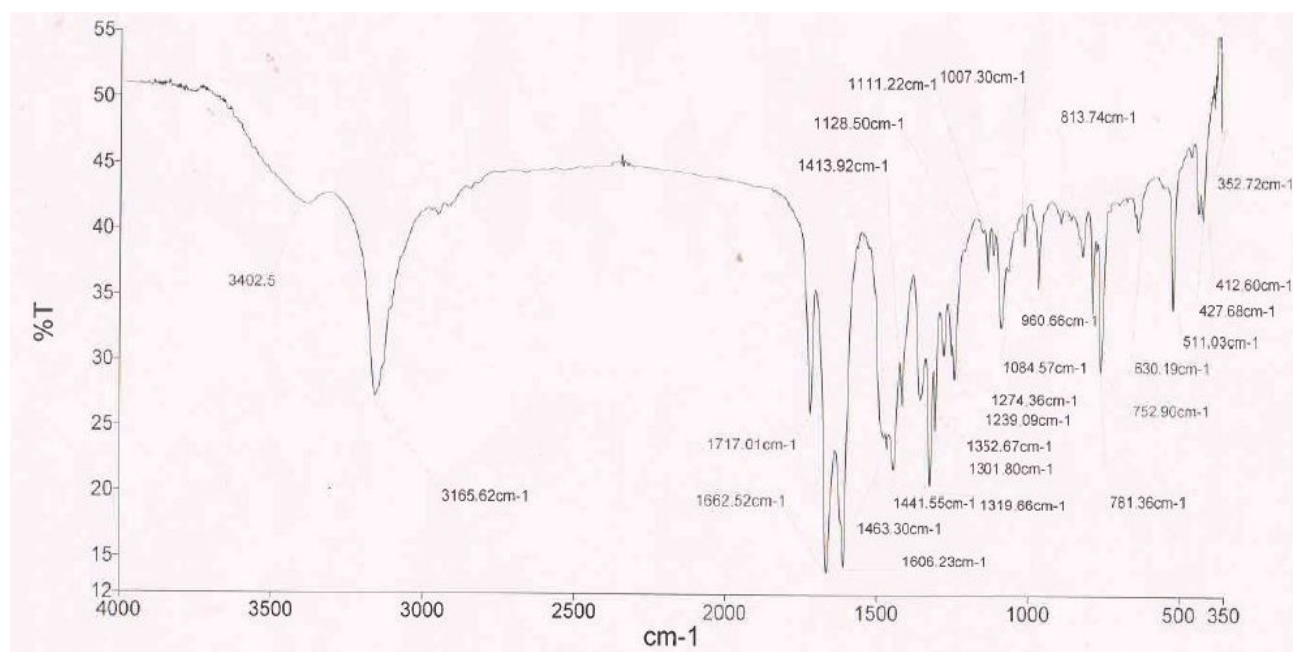


Fig.S4 IR Spectrum of $[\text{Cd}(\text{DMV})_2(\text{Benzim})_2] \cdot 2\text{H}_2\text{O}$ (**2**).

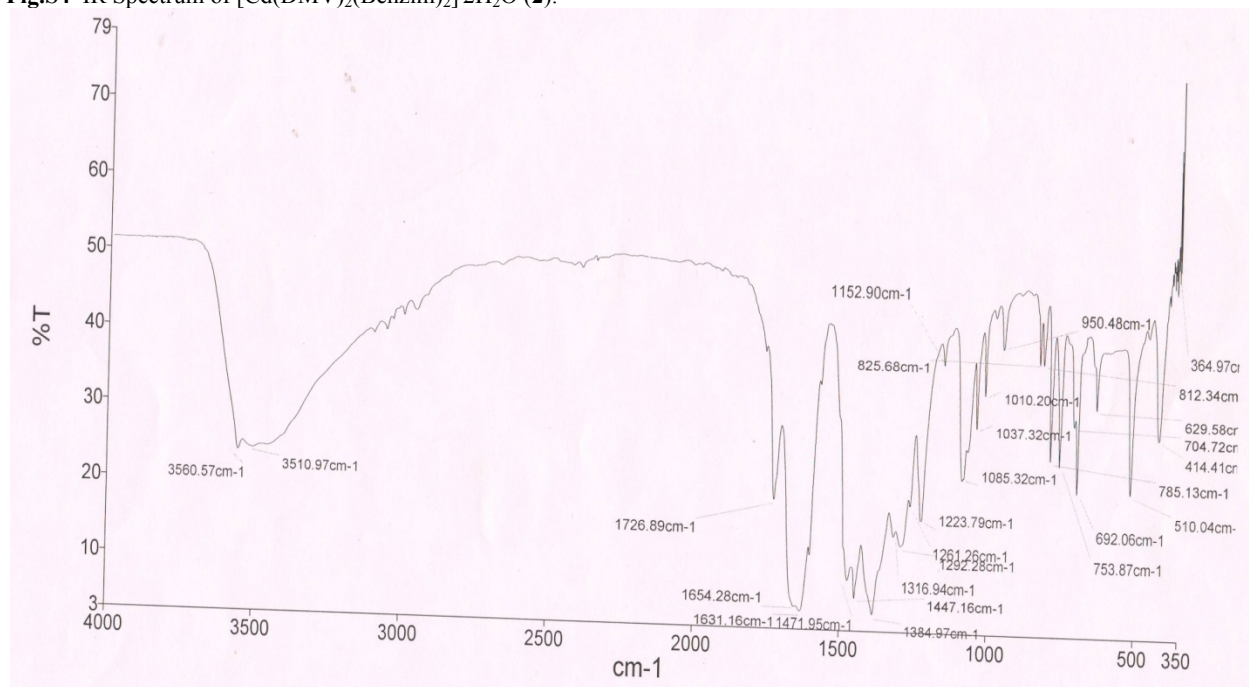


Fig.S5 IR Spectrum of $[\text{Cd}(\text{H}_2\text{O})_4(\text{py})_2](\text{DMV})_2$ (**3**)

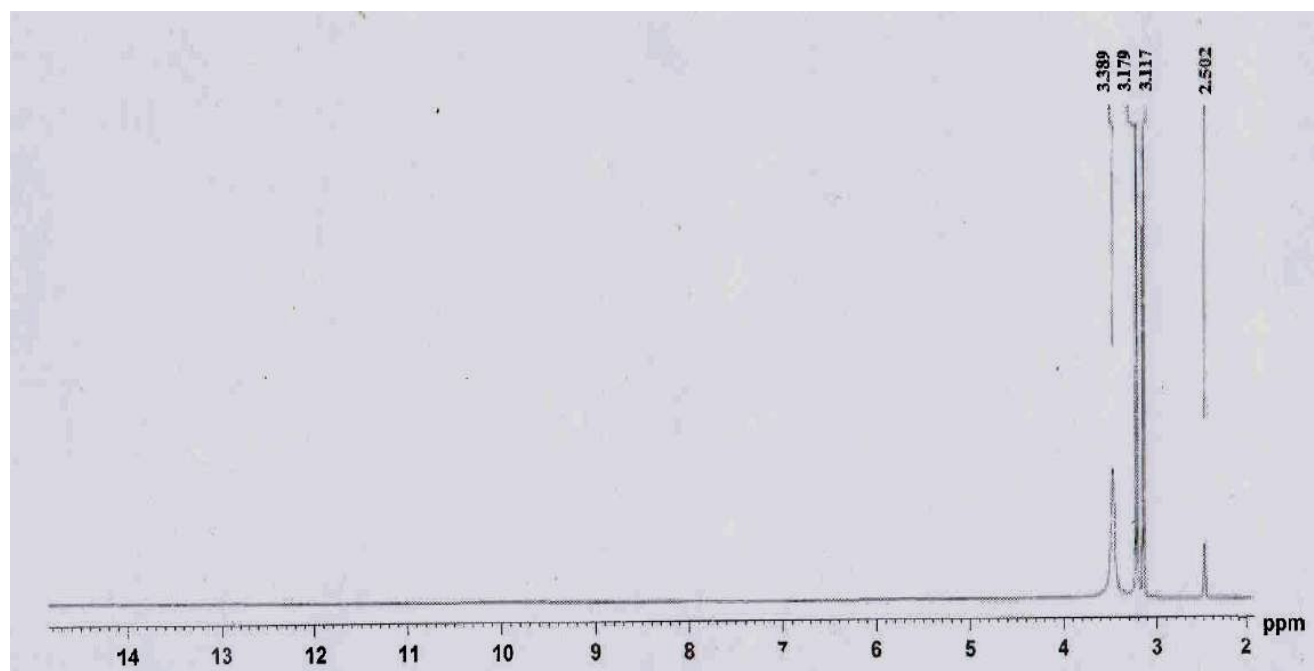


Fig.S6 ^1H -NMR Spectra of HDMV (**1**· H_2O) in $\text{DMSO}-d_6$

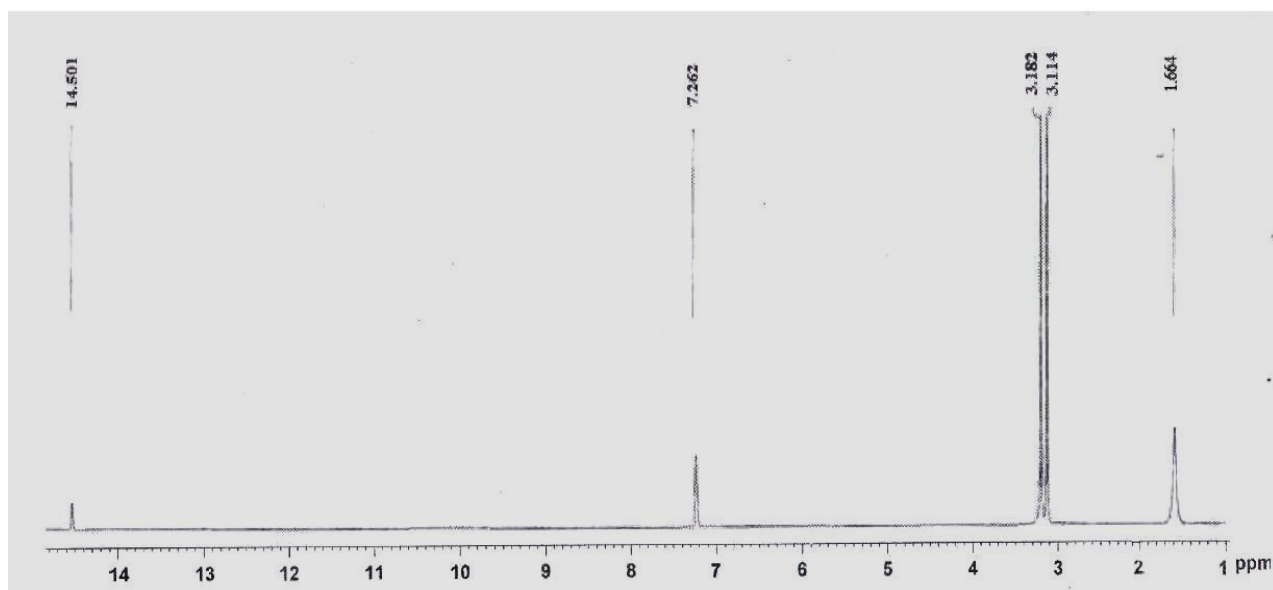


Fig.S7 ¹H-NMR Spectra of HDMV (1·H₂O) in CDCl₃

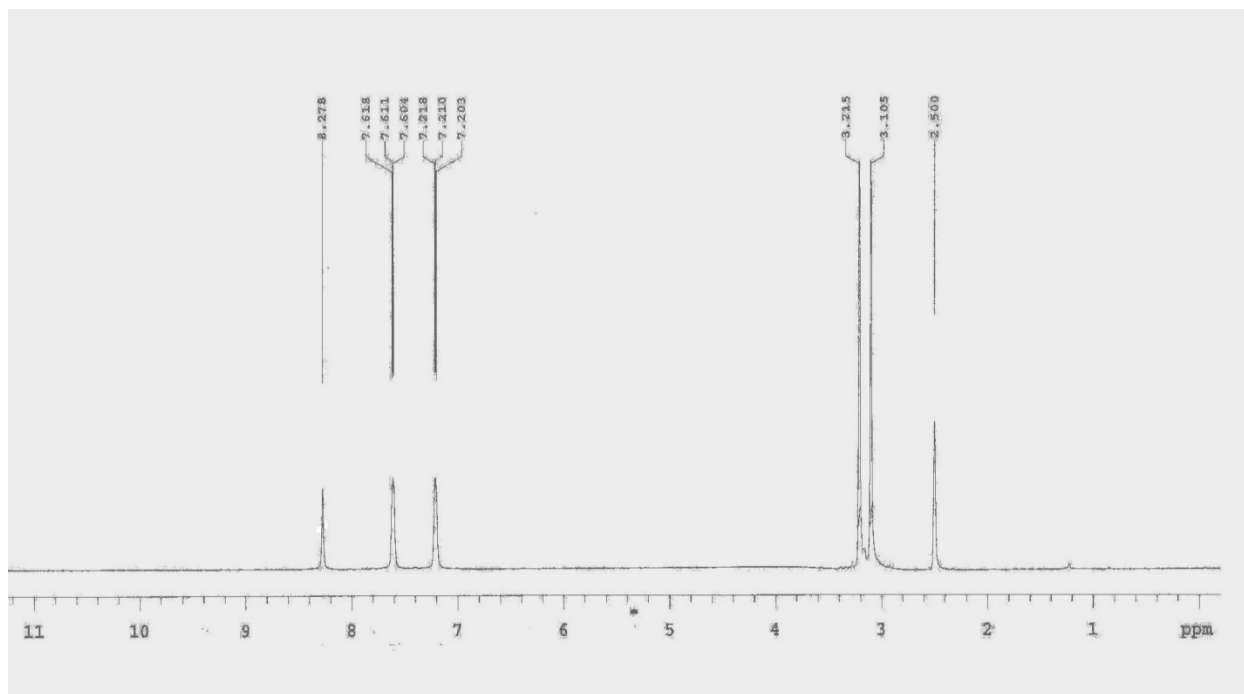


Fig.S8 ¹H-NMR Spectra of [Cd(DMV)₂(Benzim)₂]·2H₂O (2).

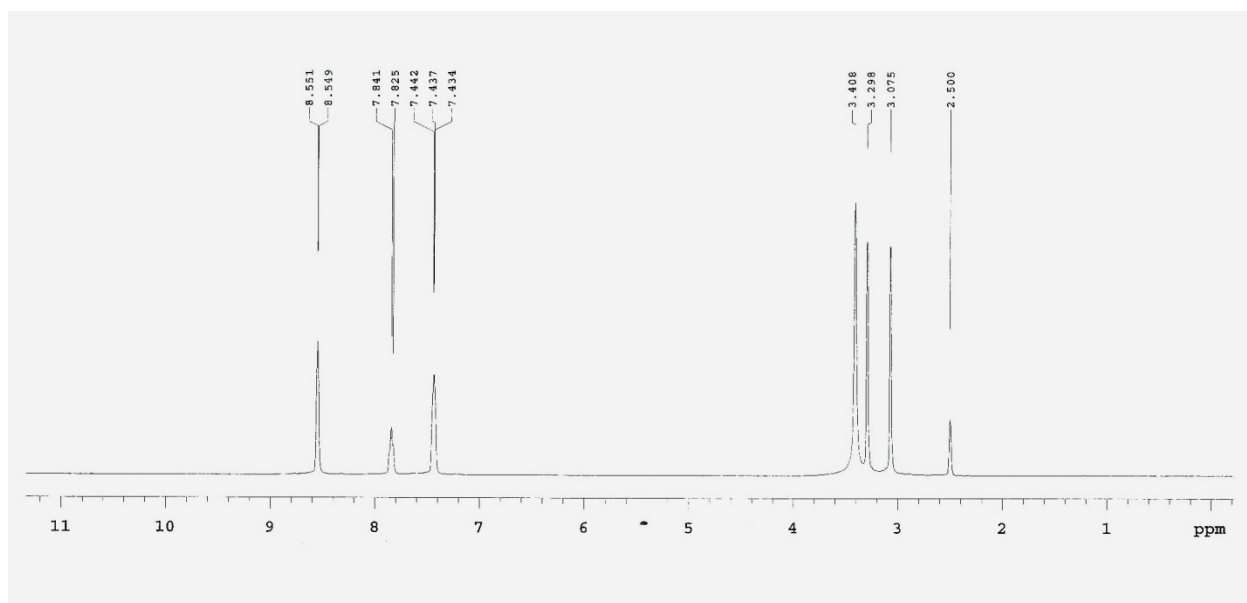


Fig.S9 ¹H-NMR Spectra of [Cd(H₂O)₄(py)₂](DMV)₂ (**3**)

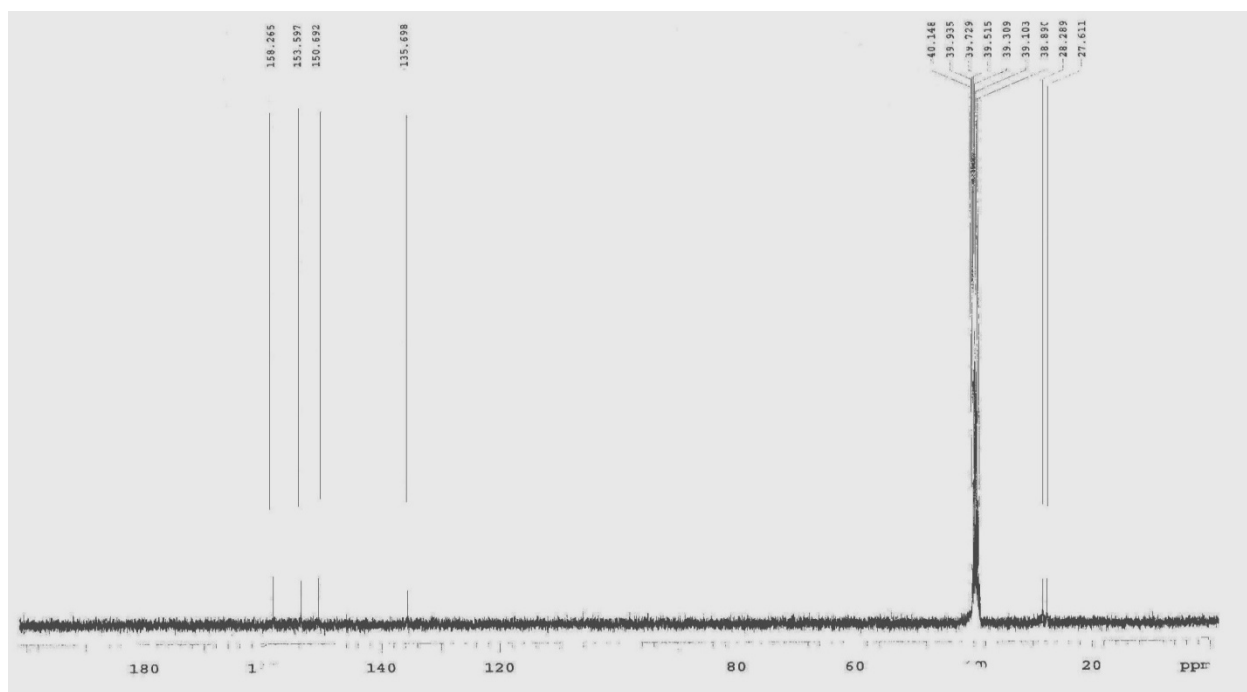


Fig.S10 ¹³C-NMR Spectra of HDMV (**1**·H₂O)

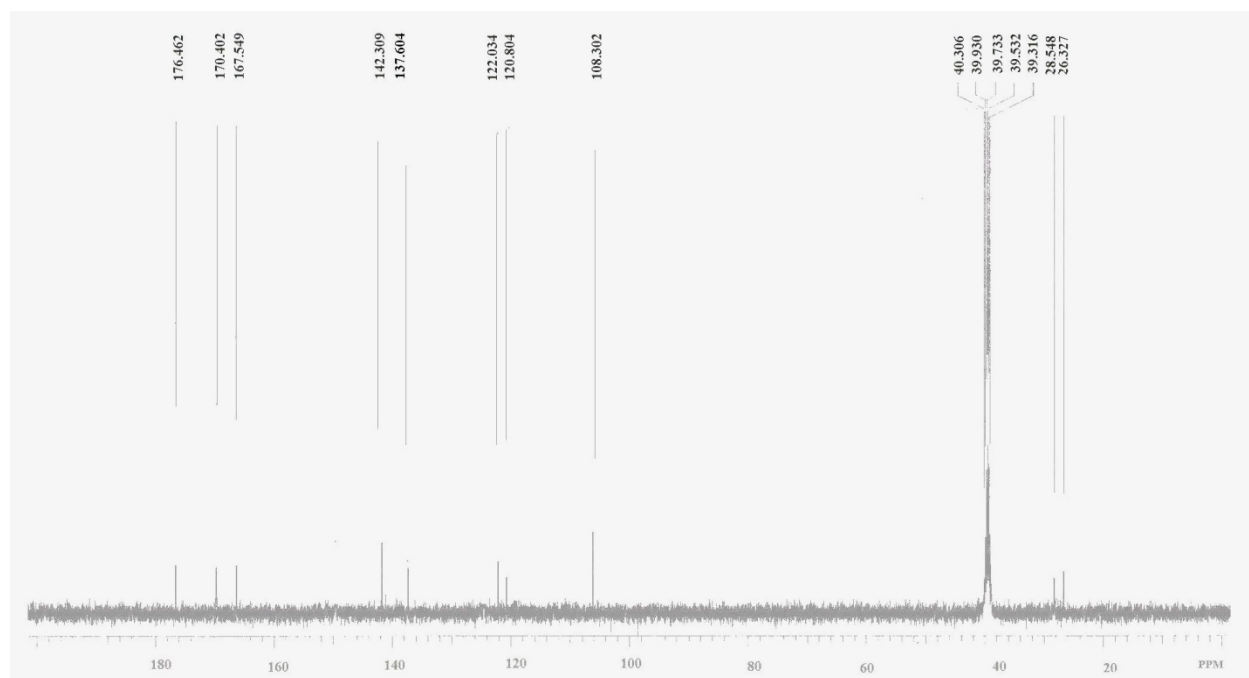


Fig.S11 ¹³C-NMR Spectra of [Cd(DMV)₂(Benzim)₂] (2)

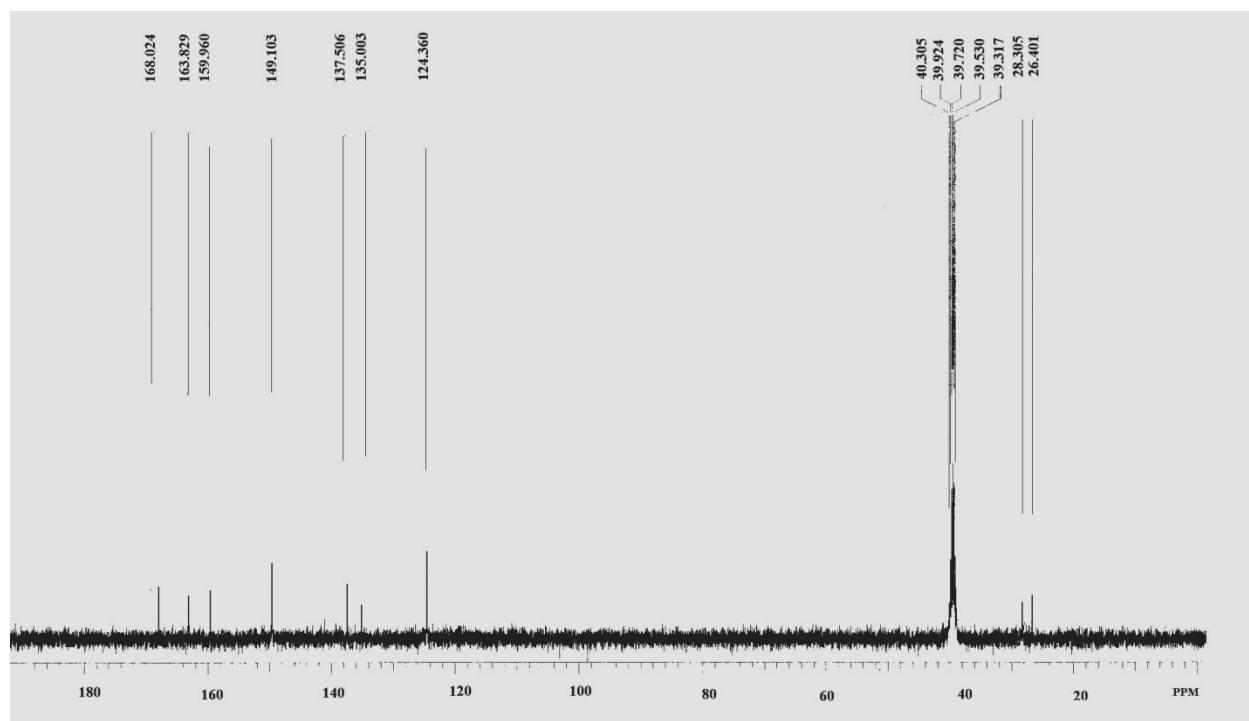


Fig.S12 ¹³C-NMR Spectra of [Cd(H₂O)₄(py)₂](DMV)₂ (3)