Electronic Supplementary Information

Syntheses, Structures and Magnetic Properties of Cyano-Bridged One-Dimensional Ln^{3+}-Fe^{3+} (Ln = La, Dy, Ho and Yb) Coordination Polymers

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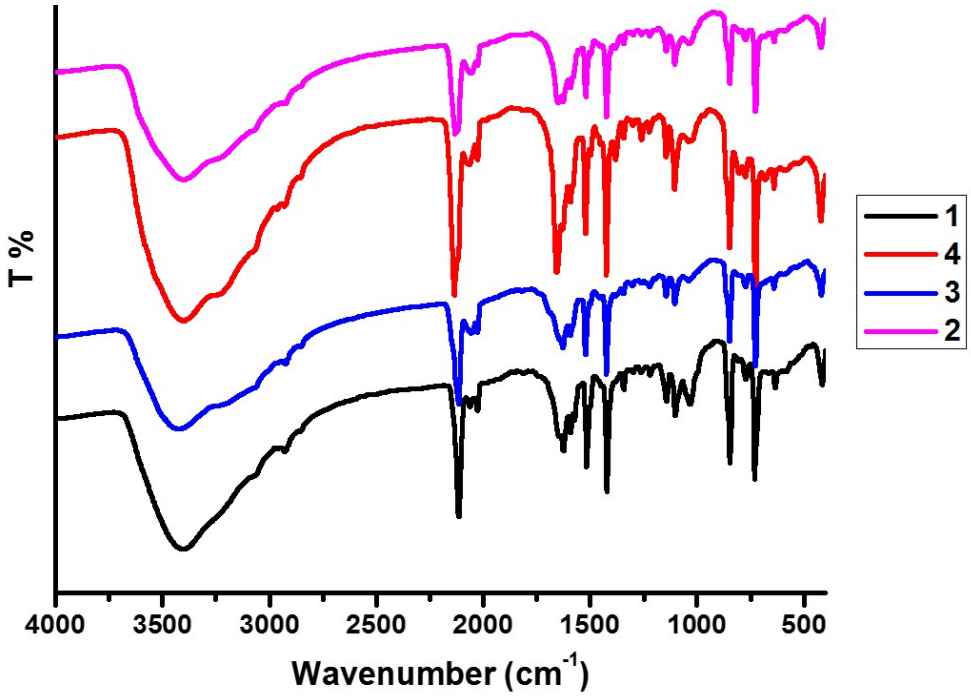

Figure S1: FT-IR spectra of **1**-**4**.

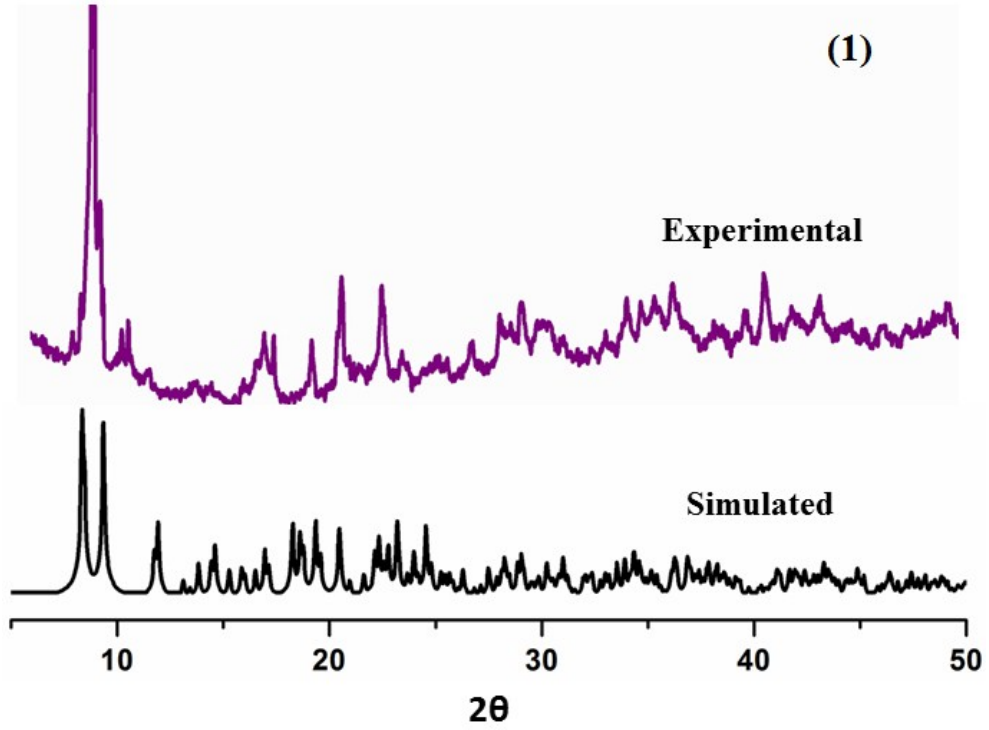

Figure S2: Simulated and experimental X-ray powder diffractogram for compound **1**.

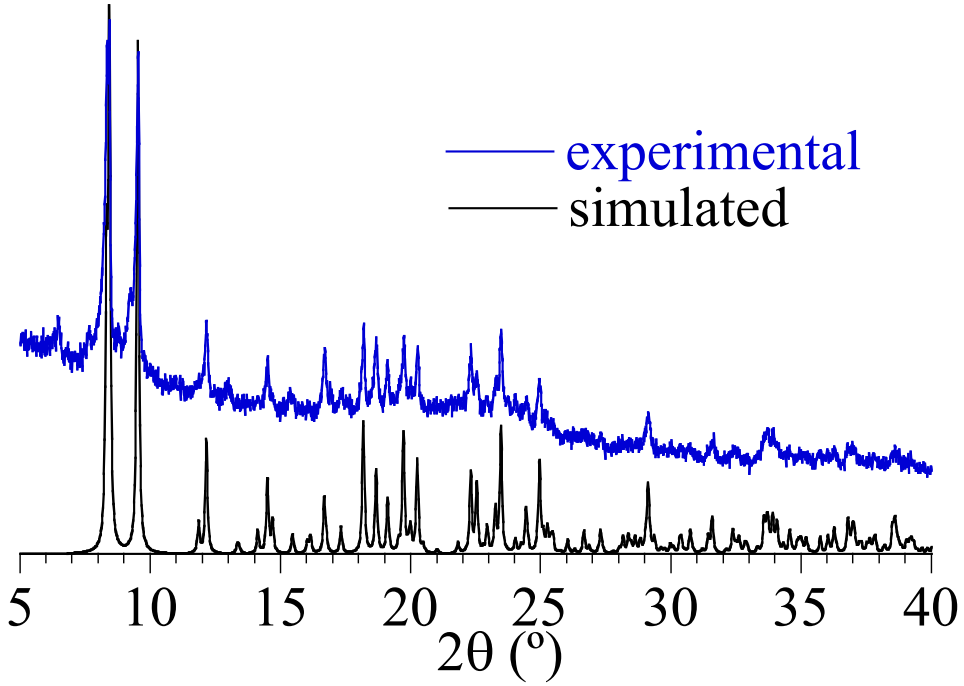

Figure S3. Simulated and experimental X-ray powder diffractogram for compound **2**.

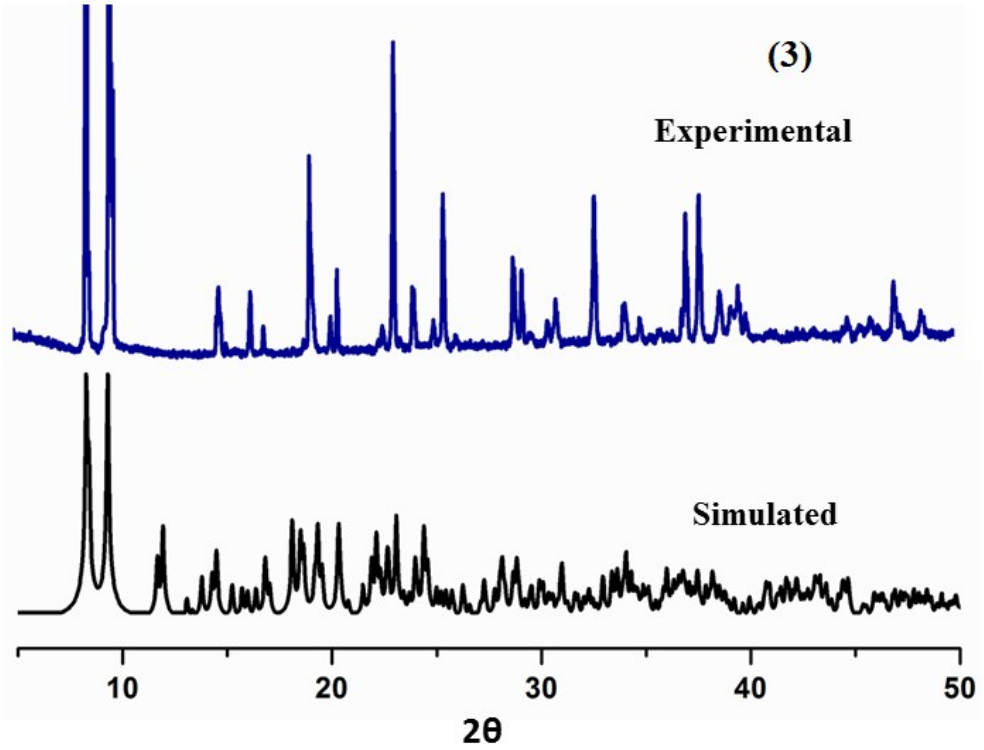

Figure S4. Simulated and experimental X-ray powder diffractogram for compound **3**.

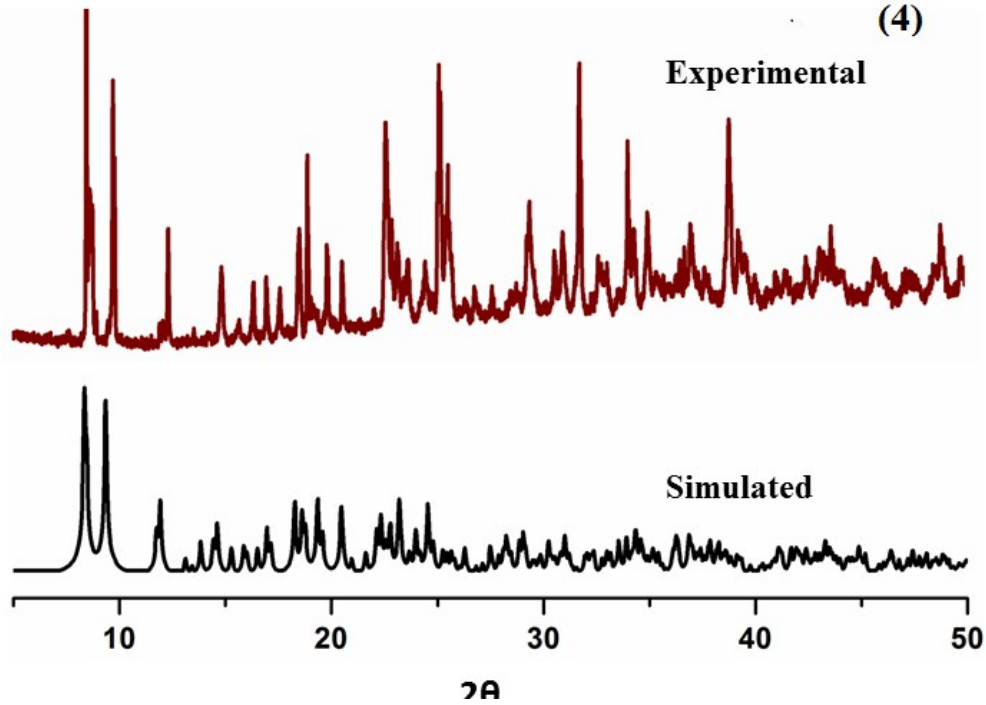

Figure S5. Simulated and experimental X-ray powder diffractogram for compound **4**.

X-ray crystallography

Suitable crystals of compounds **1-4** were selected and mounted on suitable supports on a SuperNova, Dual, Cu at zero, Eos diffractometer. The crystals were kept at a steady T = 293 K during data collection. The structures were solved with the ShelXT[1] structure solution program using the dual solution method and by using Olex2[2] as the graphical interface. The model was refined with version 2018/3 of ShelXL[1] using Least Squares minimisation. All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model.

For compounds **1**, **3** and **4**, the completion of the crystal structure determination is hampered by the presence of disordered solvent molecules. Therefore, we have included their contribution to the calculated structure factors in the least-squares refinement of the crystal structure using the mask tool of Olex2.[2] For compounds **1, 3** and **4** we have applied the mask tool solvent method as an alternative means of addressing the solvent disorder issue in order to determine the exact number of solvent molecules in the voids. In compound **1** we found a total of 134.5 electrons in a volume of 772.2 Å^3, corresponding to seven H_2O molecules per moiety. In compounds **3** and **4**, we could find six ordered water molecules per moiety and with the mask tool we found, respectively, 68.0 and 72.0 electrons in voids of 568.0 Å^3 and 428 Å^3, corresponding to one additional H_2O molecule per moiety in both compounds, resulting in a total of seven crystallization water molecules per moiety in compounds **1**, **3** and **4**. The final moiety formula are: $C_{42}H_{26}FeLaN_{12}O \cdot 7[H_2O]$ for compound **1**, $(C_{60}H_{40}Fe_2Ho_2N_{20}O_4)_{0.5} \cdot 6(H_2O) \cdot 1[(H_2O)]$ for compound **3** and $(C_{60}H_{32}Fe_2N_{20}O_4Yb_2)_{0.5} \cdot 6(H_2O) \cdot 1[(H_2O)]$ for compound **4**.

A summary of the data collection and structure refinements for compounds **1-4** is given in Table 1. Crystallographic data for the structures reported in this paper have been deposited in the Cambridge Crystallographic Data Centre as a supplementary publication no. CCDC 1054136-1054139. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB21EZ, UK (fax: + (44)1223-336-033; email: deposit@ccdc.cam.ac.uk).

Table S1. Hydrogen bond distances [Å] and angles [°] in compound **2**.

D-H···A	D-H	D···A	H···A	∠D-H···A
O1^{iv}-H1A···O1W	0.884	2.710	2.095	125.96
O1-H1B···O3W	0.883	2.731	2.001	139.06
O3W^{i}-H3WA···O2W	0.850	2.765	1.964	156.71
O3W-H3WB···O4W^{ii}	0.850	2.780	1.994	153.27
O1W-H1WB···O3W^{iii}	0.849	2.841	2.074	149.90
O2W-H2WA···N4	0.850	2.890	2.289	127.88
O4W-H4WA···N5	0.850	2.961	2.132	164.76
O4W-H4WB···N4	0.851	2.973	2.127	172.67
O2W-H2WB···N5	0.851	2.998	2.151	173.78

Symmetry operations: i = 1-x,y,1/2-z; ii = 1.5-x,1/2-y,1-z;
iii = x,-y,1/2+z; iv = 1-x,y,1/2-z;

References

1. Sheldrick, G.M., Crystal structure refinement with ShelXL, *Acta Cryst.*, (2015), C71, 3-8.

2. O.V. Dolomanov and L.J. Bourhis and R.J. Gildea and J.A.K. Howard and H. Puschmann, Olex2: A complete structure solution, refinement and analysis program, *J. Appl. Cryst.*, (2009), **42**, 339-341.