Supplementary Material (ESI) for CrystEngComm

Supplementary informations

$[Fe(phen)(CN)_4]^-$: a suitable metalloligand unit to build 3*d*-4*f* heterobimetallic complexes with mixed bpym-cyano bridges (phen = 1,10-phenantroline, bpym = 2,2'-bipyrimidine)

Diana Visinescu, Oscar Fabelo, Catalina Ruiz-Pérez, Francesc Lloret and Miguel Julve

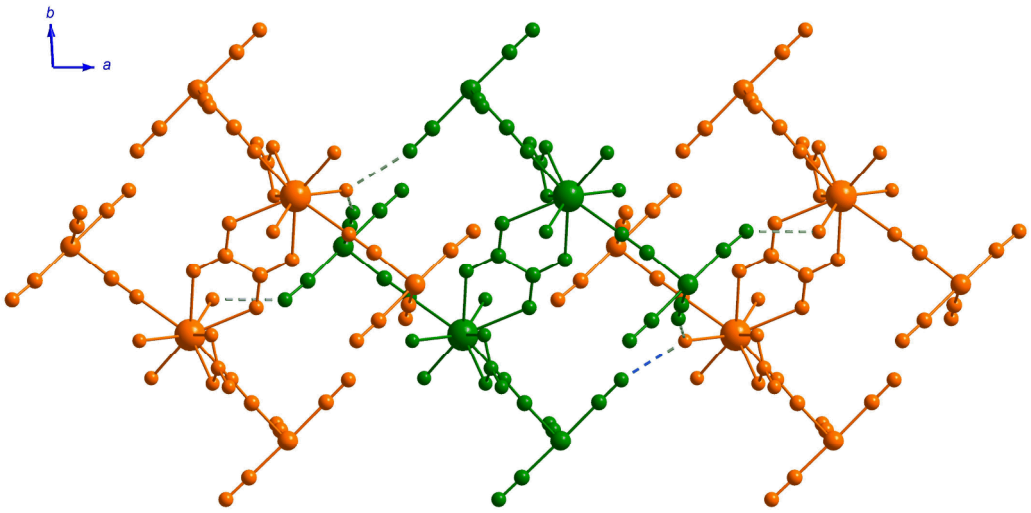

Fig. S1 A detail of the crystal packing in **1, 3** and **4** showing the supramolecular channels along *a* axis, through N···O type hydrogen bonds (blue dashed lines). Each hexanuclear unit is represented in a different colour and the bpym ligand has been simplified for clarity.

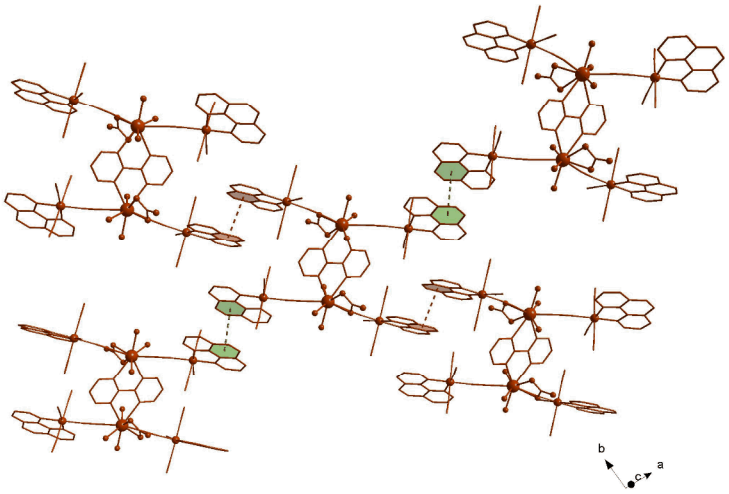

Fig. S2 A view of the inter-ring type interactions in **1**, **3** and **4**, revealing the two sets of the slipped-off π-π stacking contacts (brown and green dashed lines).

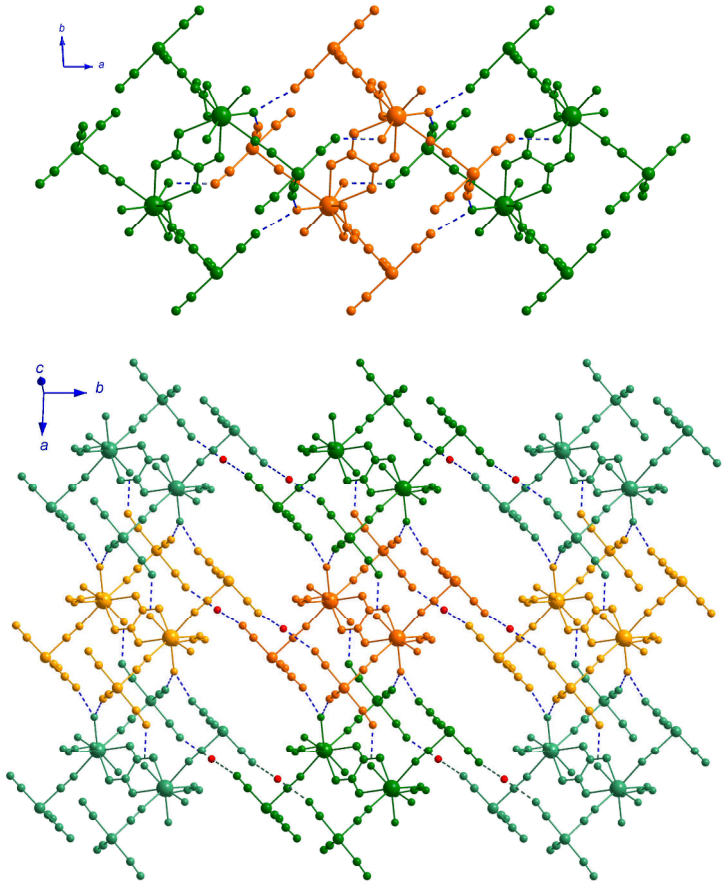

Fig. S3 (Top) A perspective view of the chains of hexanuclear of **2** running along the *a* axis. (Bottom) A view in the *ab* plane of the interchain linking in **2** via hydrogen bonds involving the O(5W) water molecules (red spheres). The phen molecule and part of the carbon atoms of the bpym bridging ligand have been omitted for the sake of the clarity.

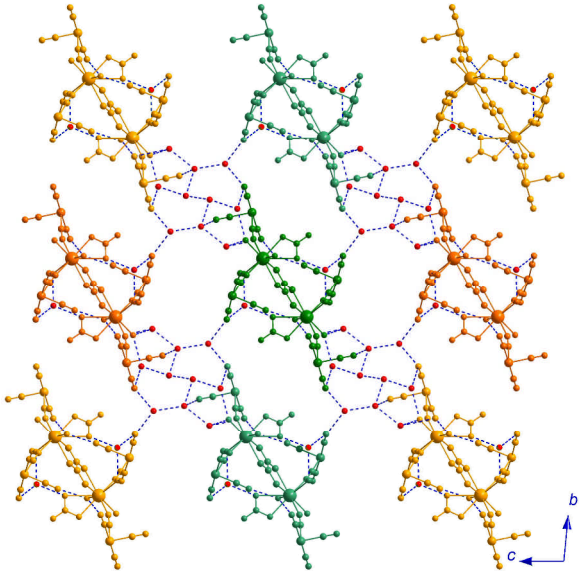

Fig. S4 Details of the crystal packing in **2** showing the hydrogen-bonding pattern which links the supramolecular channel