Electronic Supplementary Material (ESI) for Dalton Transactions

Supplementary Information

In situ ligand formation in the synthesis of an octanuclear dysprosium 'double cubane' cluster displaying single molecule magnet features

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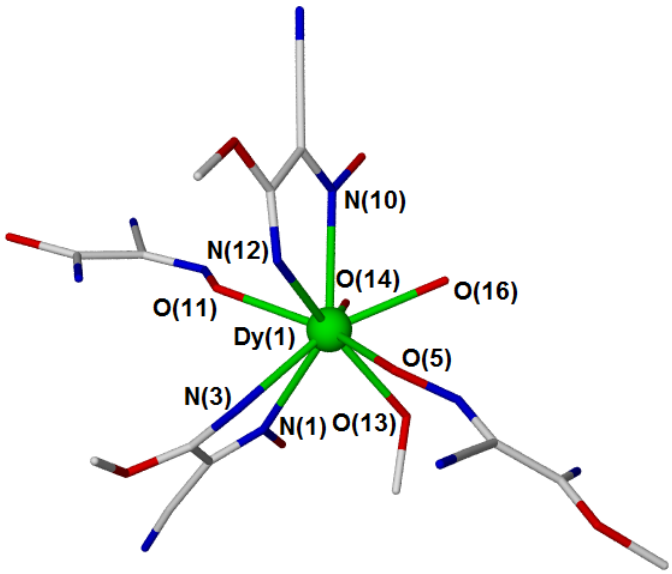
(a)



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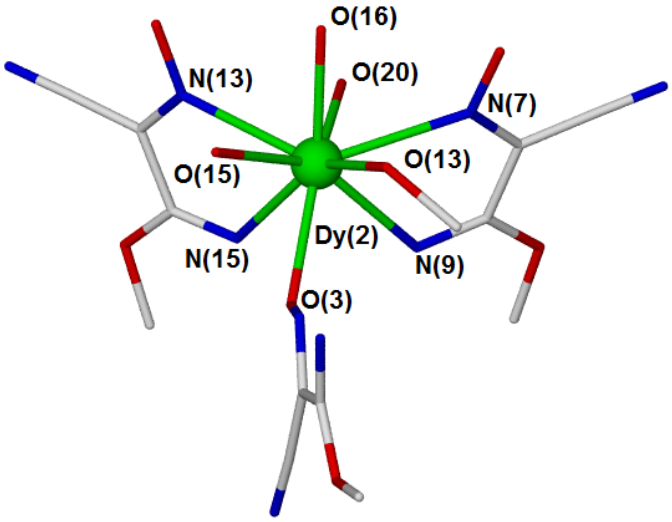

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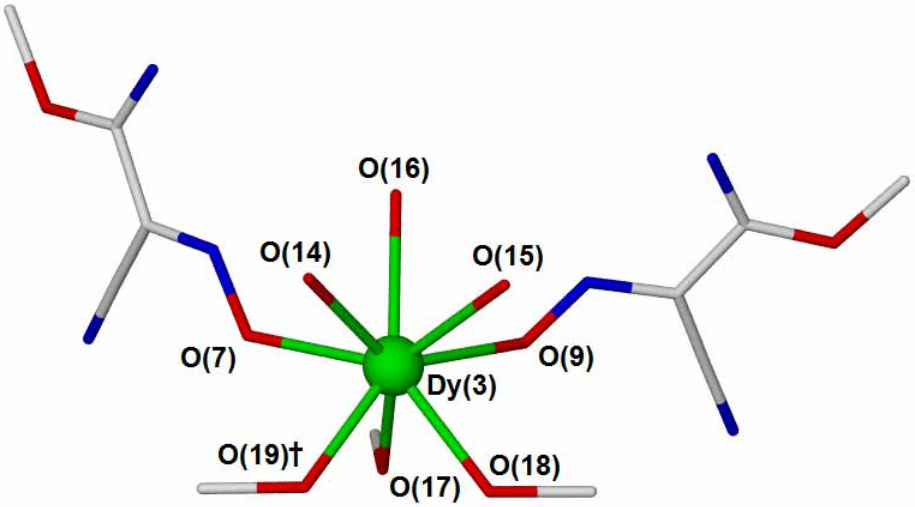

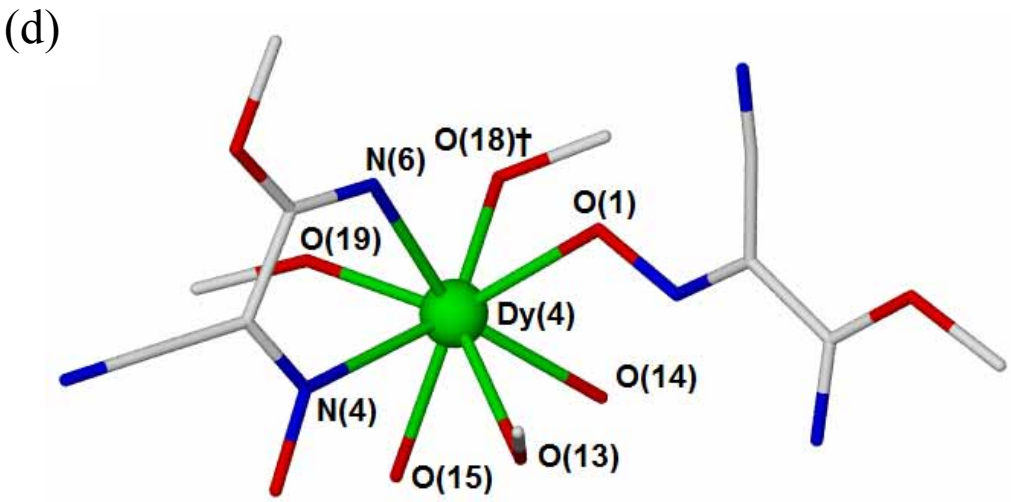

Fig. S1 The coordination environments of the four unique dysprosium atoms in complex **1**. Symmetry element used: † = 1 − x, 1 − y, −z. Hydrogen atoms omitted for clarity.

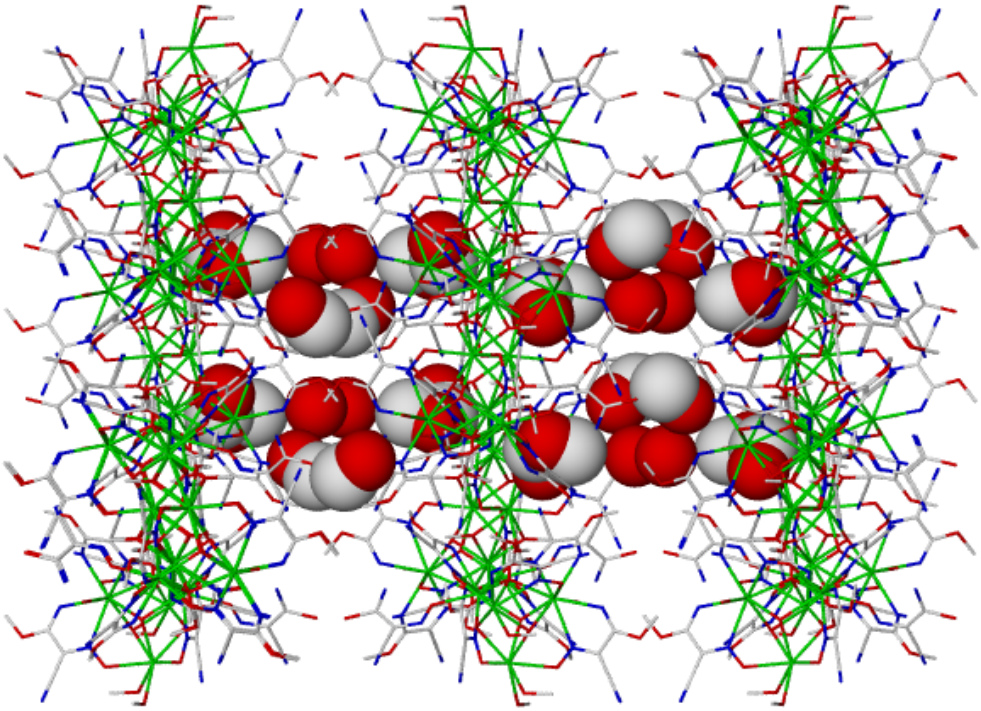

Fig. S2 $[Dy_8(OH)_6(OMe)_6(cmnm)_{10}(ccnm)_2(H_2O)_2(MeOH)_2]\cdot 2H_2O\cdot 6MeOH$ (**1**$\cdot 2H_2O\cdot 6MeOH$) as viewed down *a*-axis. Lattice methanol molecules emphasised. Hydrogen atoms omitted for clarity.

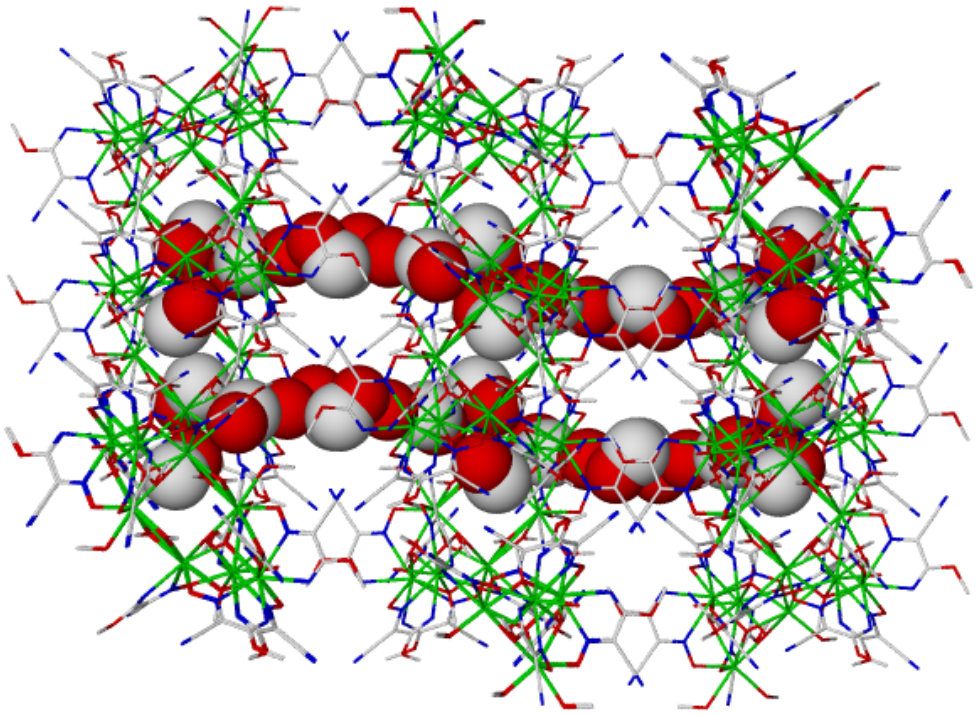

Fig. S3 $[Dy_8(OH)_6(OMe)_6(cmnm)_{10}(ccnm)_2(H_2O)_2(MeOH)_2]\cdot 2H_2O\cdot 6MeOH$ (**1**$\cdot 2H_2O\cdot 6MeOH$) as viewed down *b*-axis. Lattice molecules emphasised. Hydrogen atoms omitted for clarity.

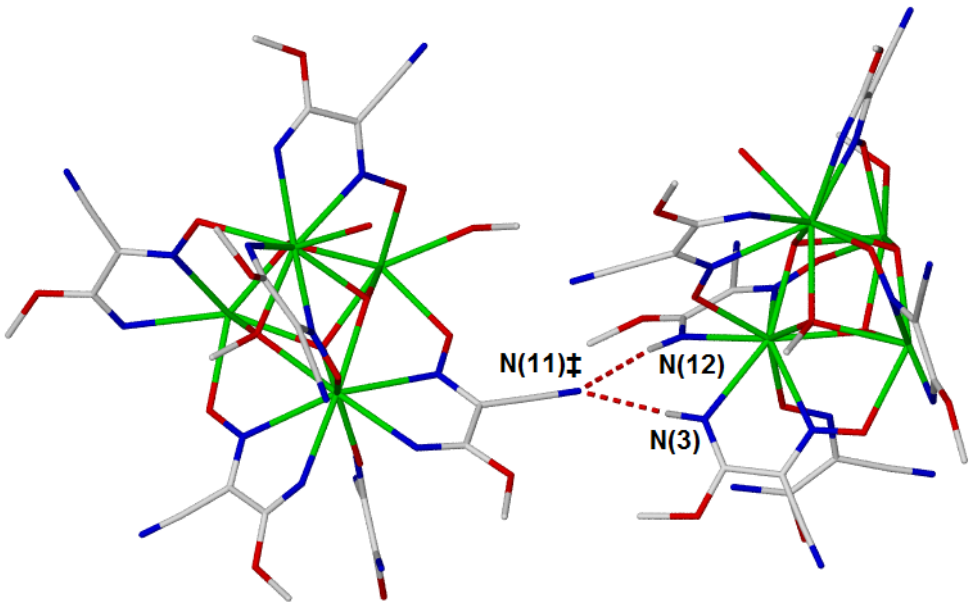

Fig. S4 The nitrogen atoms of two imine groups of two cmnm ligands acting as hydrogen bond donors to a nitrile group of a cmnm ligand of an adjacent complex. Non-hydrogen bonding hydrogen atoms omitted for clarity. Symmetry element used: ‡ = $^3/_2$ – x, y, $^1/_2$ + z.

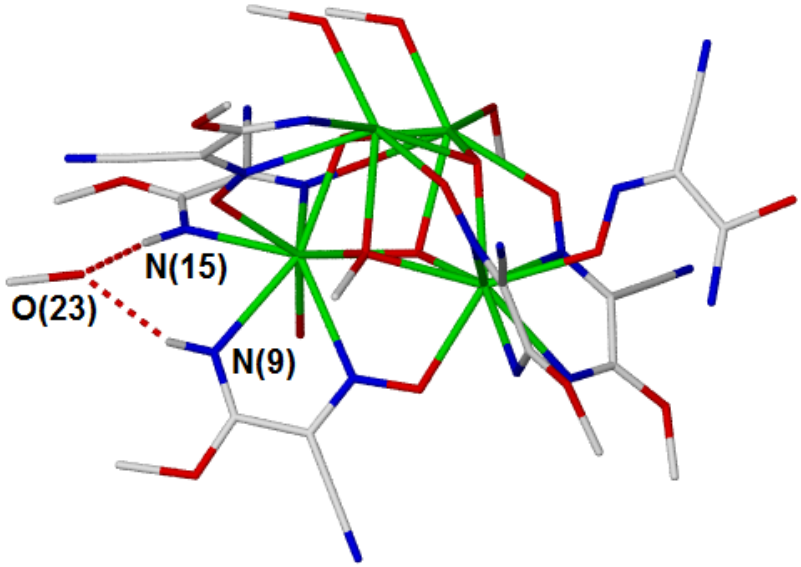

Fig. S5 The nitrogen atoms of two imine groups of two cmnm ligands acting as hydrogen bond donors to a methanol molecule in the lattice. Non-hydrogen bonding hydrogen atoms omitted for clarity.

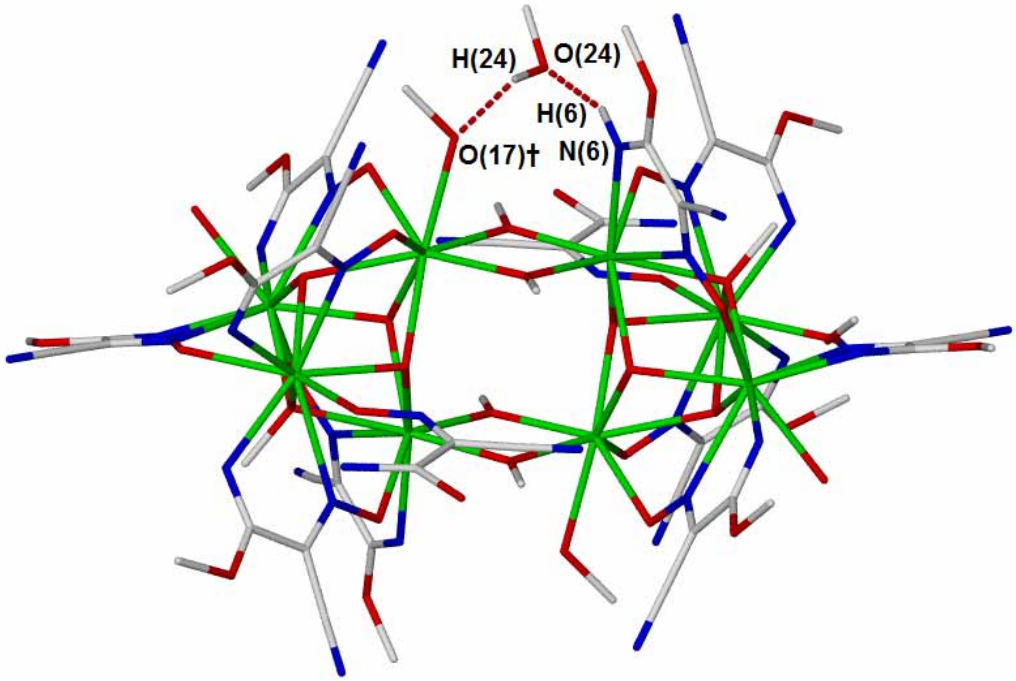

Fig. S6 An imine group of a cmnm ligand acting as a hydrogen donor to a lattice methanol molecule, which in turn is a hydrogen bond donor to a coordinated methanol molecule. Non-hydrogen bonding hydrogen atoms omitted for clarity. Symmetry element used: † = 1 − x, 1 − y, −z.

Table S1 Hydrogen bond lengths (Å) and angles (°) of **1**.[a]

N(12)···N(11)‡	3.134(8)	N(12)–H(12)···N(11)‡	170.2
N(3)···N(11) ‡	3.190(9)	N(3)–H(3)···N(11)‡	158.3
N(9)···O(23)	2.914(9)	N(9)–H(9)···O(23)	153.8
N(15)···O(23)	2.907(8)	N(15)–H(15)···O(23)	155.9
N(6)···O(24)	2.818(10)	N(6)–H(6)···O(24)	147.6
O(24)···O(17)†	2.864(9)	O(24)–H(24)···O(17)†	157.5

[a] Symmetry elements used: ‡ = $^3/_2$ – x, y, $^1/_2$ + z; † = 1 − x, 1 − y, −z.

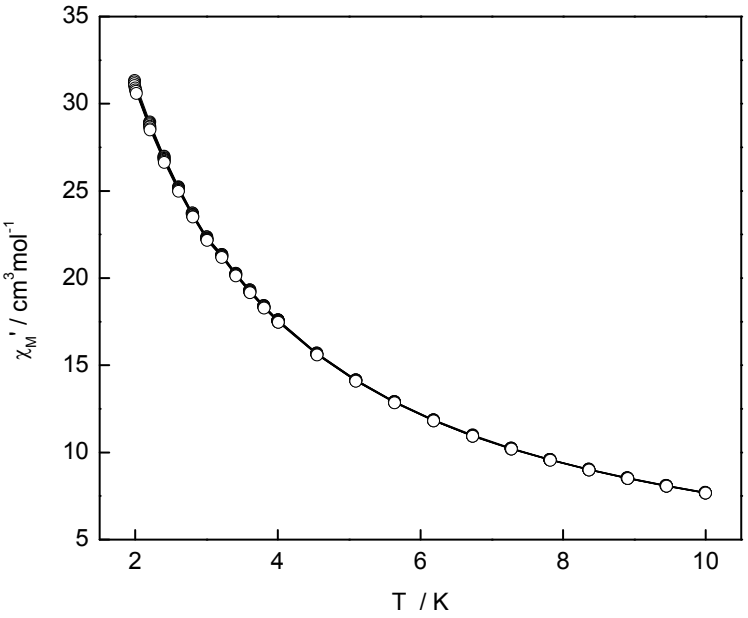

Fig. S7 Plots of ac in-phase susceptibilities, $\chi_{M'}$, for **1** using the frequencies given in the text (Experimental)