

## ELECTRONIC SUPPLEMENTARY INFORMATION

to

### **A triacontanuclear [Zn<sub>12</sub>Dy<sub>18</sub>] cluster: a ring of [Dy<sub>4</sub>] cubes†**

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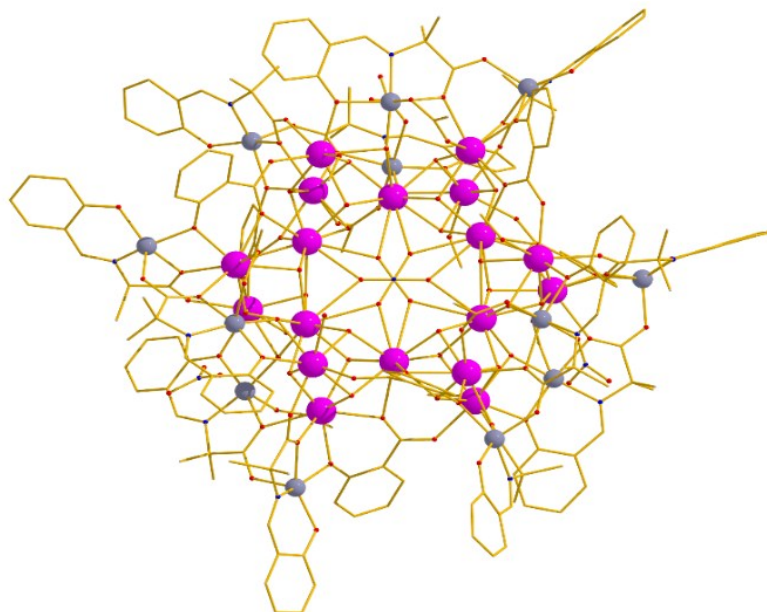
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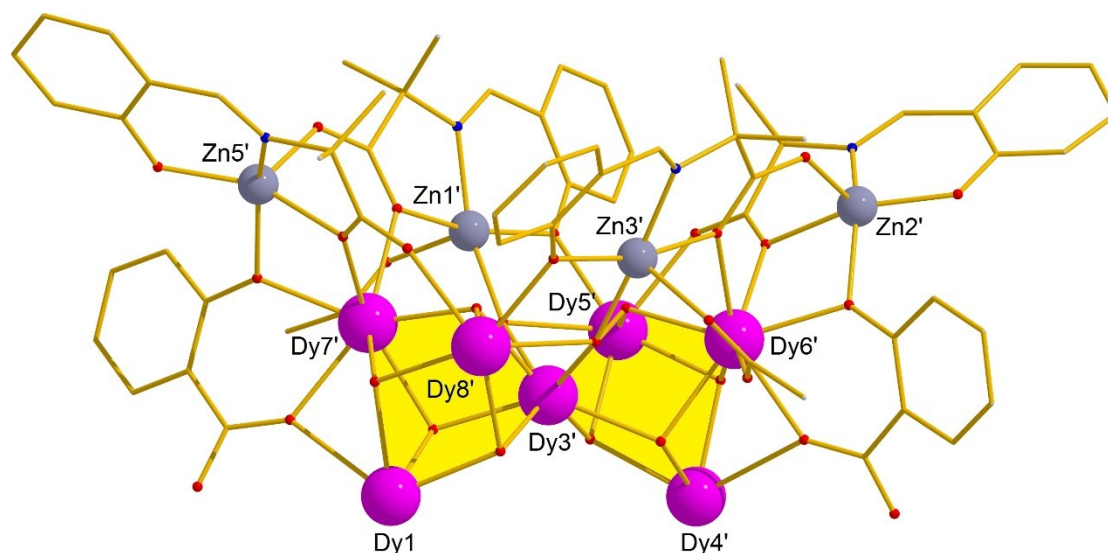
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### Elemental Analysis for complex 1.

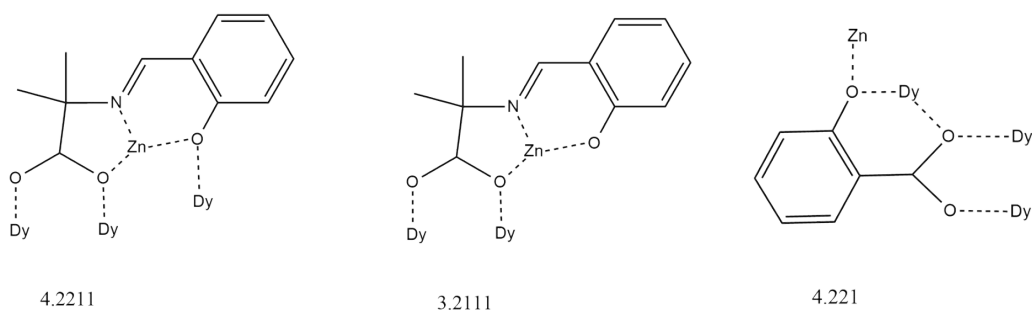
C, H, N analysis: Anal. Calcd for  $C_{191}H_{232}Dy_{18}N_{18}O_{123}Zn_{12}$  ( $1 \cdot 3MeOH \cdot 2H_2O$ ): C, 27.12; H, 2.76; N, 2.98%. Found: C, 27.26 H, 2.49 N 2.87%.



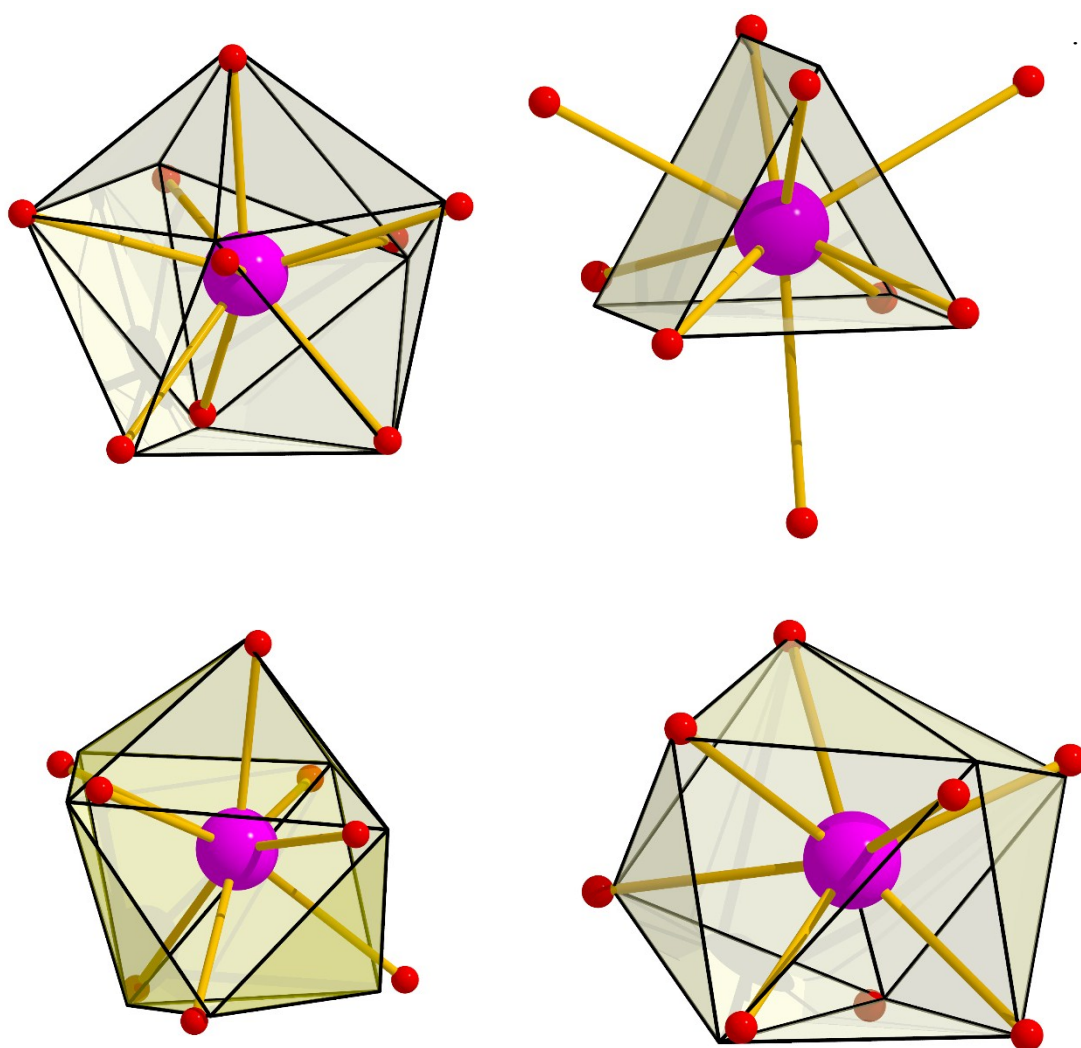
**Fig. S1** The molecular structure of the cation of **1** in top-view. Colour code:  $Zn^{II}$  = blue-grey,  $Dy^{III}$  = pink, O = red, N = blue, C = white.



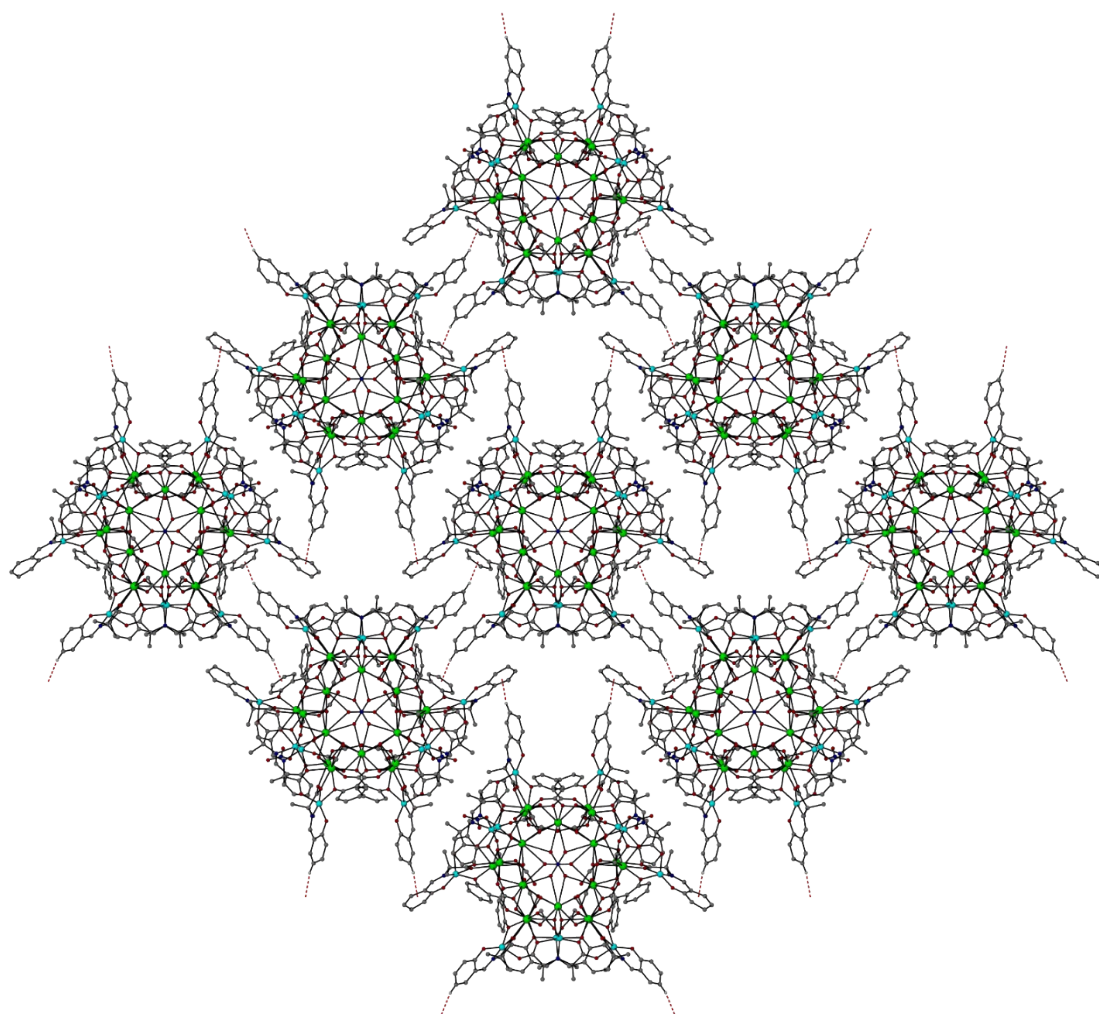
**Fig. S2** The binding of four  $Zn^{II}$  atoms on a dimer of  $[Dy_4(OH)_4]$  cubes, for the formation of a  $\{Dy_7Zn_4(OH)_{10}(L)_4(sal-COO)_2(OAc)_2\}$  bowl-shaped unit. Colour code:  $Zn^{II}$  = blue-grey,  $Dy^{III}$  = pink, O = red, N = blue, C = white.



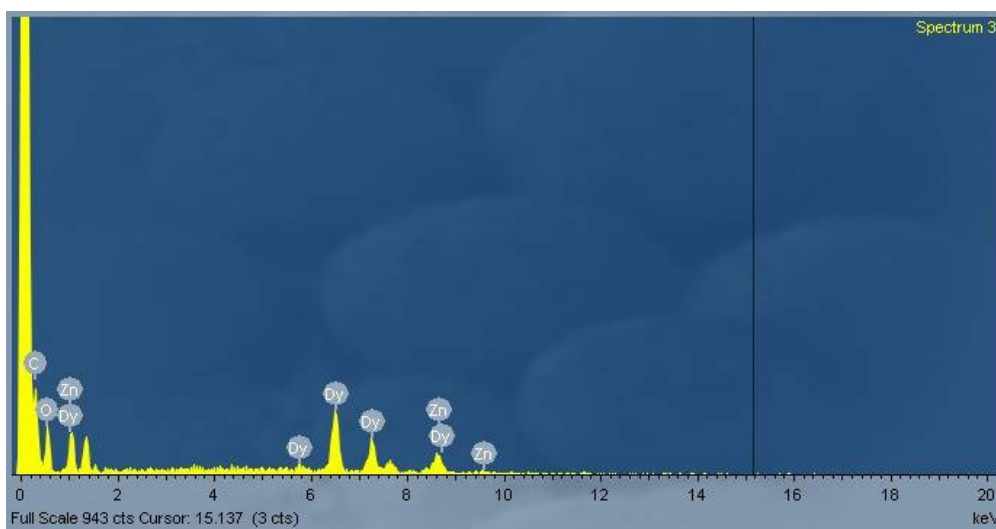
**Fig. S3** The coordination modes of the dianion of the Schiff base ligand made *in situ* between salicylaldehyde and aibH,  $L^{2-}$  (left and center) and the salicylate dianion (right)



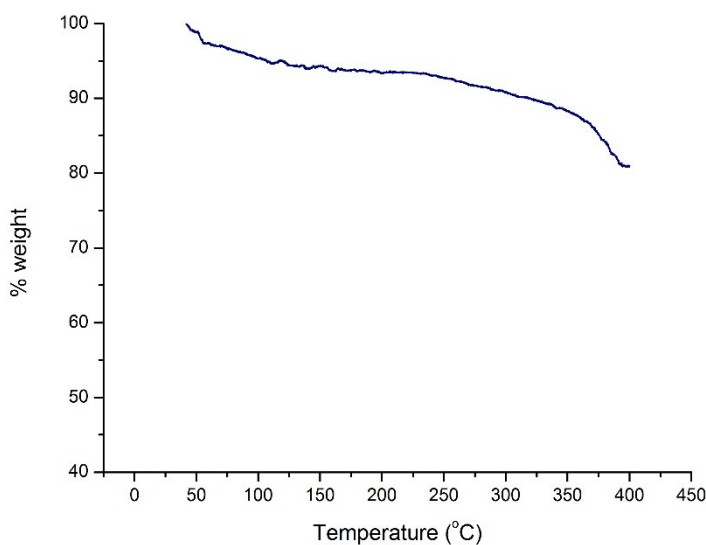
**Fig. S4** The coordination geometries of representative  $Dy^{III}$  metal centers:  $Dy_3$  (spherical tricapped trigonal prism; top-left),  $Dy_4$  (tricapped trigonal prism; top-right),  $Dy_7$  (square antiprism; bottom-left) and  $Dy_{10}$  (triangular dodecahedron; bottom-right).



**Fig. S5** The square grid of clusters parallel to the (1, 0, -1) plane. All hydrogen atoms, except those participating in the weak interactions, have been removed. C-H $\cdots$  $\pi$  interactions are shown as dashed red lines. Color code: C gray, H white, N blue, O red, Dy green, Zn cyan.

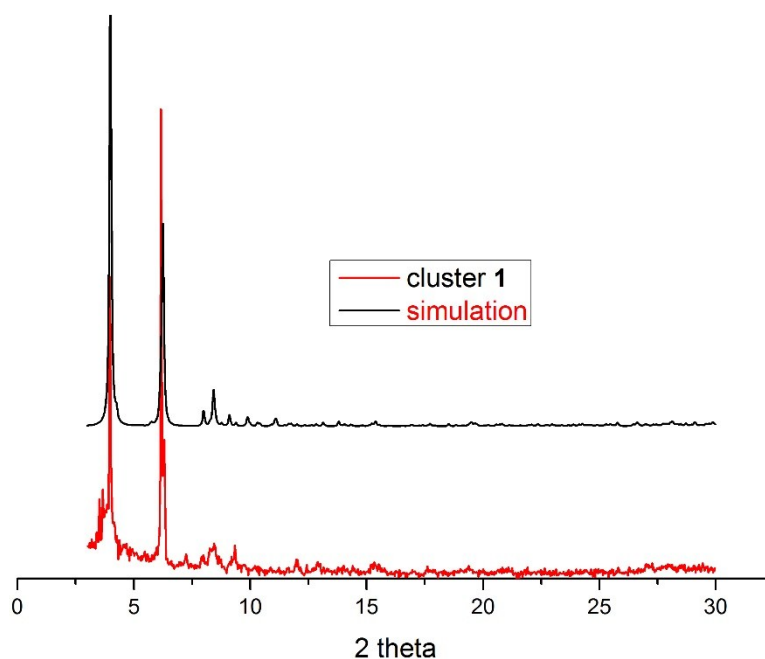


**Fig. S6** EDS analysis of cluster **1**, yielding a Zn : Dy ratio of 0.654, in excellent agreement with the theoretical value of 0.666 (2:3) expected from the crystal structure.

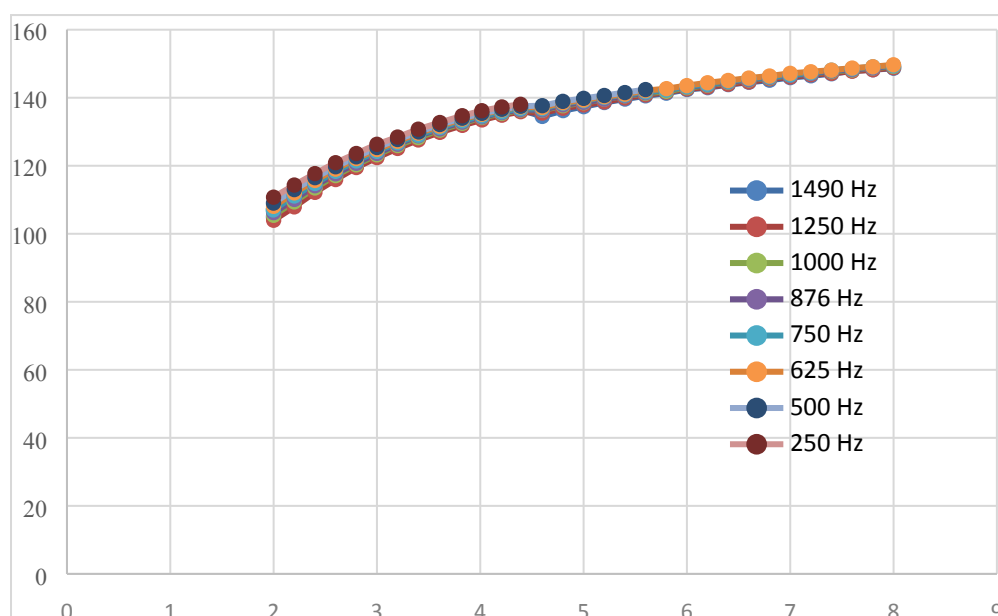


**Fig. S7** TGA analysis of cluster **1** in the 40 – 400 °C temperature range; The thermal decomposition of complex **1**·12MeOH·5H<sub>2</sub>O starts with a weight loss of ~4.5% in the 40–90 °C region, corresponding to the loss of 12 moles of MeOH per mole of complex **1**·12MeOH·5H<sub>2</sub>O (theoretical loss of 4.4%), while upon further heating to ~110 °C further weight loss of ~ 1.1 % is observed, corresponding to the loss of 5 moles of H<sub>2</sub>O per mole of complex **1**·12MeOH·5H<sub>2</sub>O (theoretical loss of 1.0%). Upon further heating to ~130 °C a small weight loss of ~ 1.0 % is observed, corresponding to the loss of 6 moles of H<sub>2</sub>O (coordinated ones) per mole of complex

**1**·12MeOH·5H<sub>2</sub>O (theoretical loss of 1.2 %). The fragment remains “stable” until ~ 250 °C, while heating above 250 °C leads to thermal decomposition.



**Fig. S8** Powder XRD diagrams' comparison between **1** and its simulated pXRD diagram. The difference in the peaks' intensity is due to preferred orientation. We have encountered no problems at all with the reproducibility of the cluster in pure crystalline form.



**Fig. S9** Plot of the in-phase  $\chi_M' T$  signals for **1** in ac susceptibility studies vs.  $T$  in a 3.5 G oscillating field at the indicated frequencies, under zero static field.