New structural form of a Tetranuclear Lanthanide Hydroxo Cluster: Dy$_4$ Analogue display Slow Magnetic Relaxation

Ananda Kumar Jami,a Viswanathan Baskar⁎a, E. Carolina Sañudo b

a School of Chemistry, University of Hyderabad, Hyderabad 500046, India

b Departament de Química Inorgànica i Institut de Nanociència i Nanotecnologia, Universitat de Barcelona, Diagonal 645 08028, Barcelona, SPAIN.

vbsc@uohyd.ernet.in

Supplementary Information

Ortep diagrams for compound 2-3: 1
(All structures with thermal ellipsoids shown at 30% probability.)

IR spectra for 1-3: 2-5
PXRD patterns for 1-3: 6-7
TGA plots for 1-3: 8
**Figure S1:** The solid state structure of 2 hydrogen atoms and solvents of crystallization are omitted for clarity.

**Figure S2:** The solid state structure of 3 hydrogen atoms and solvents of crystallization are omitted for clarity.
IR spectra of compound 1:
IR spectra of compound 2:
Note: In the IR spectra of compounds 1-3, Broad peak around 3400 cm$^{-1}$ indicates the presence of hydroxyl groups. Peak around 1630 cm$^{-1}$ indicates presence of coordinated imine nitrogens (−C=N). A peak at around 1220 cm$^{-1}$ indicates (−C-O) coordination through the phenolic oxygen atom.
PXRD patterns for compound 1-3:

To ensure the phase purity of the compounds 1-3, X-ray powder diffraction studies for all the compounds have been performed and compared to the simulated patterns obtained from the single crystal X-ray analysis.
Compound 3

Experimental
Simulated

2 $\Theta$ (degree)
Figure S3: Thermo gravimetric plots for compound 1-3.

TGA studies were carried out under flow of N₂ at heating rate of 10°C min⁻¹ for crystalline compounds 1-3 in the temperature range 30 - 800°C. All the compounds show weight loss from the approximately 80°C, followed by continuous decomposition.