

ELECTRONIC SUPPLEMENTARY INFORMATION

to

Dodecanuclear $[\text{Ni}^{\text{II}}_8\text{Ln}_4]$ clusters: rings of corner-sharing $\{\text{M}_2\text{Ln}_2\}$ cubanes ($\text{M} = \text{Ni}^{\text{II}}$; $\text{Ln} = \text{Dy, Gd, Y}$)

Thomas G. Tziotzi,^a Eleftheria Agapaki,^b Emmanouil K. Charkiolakis,^c David Gracia,^c Marc Ubach I Cervera,^c Scott J. Dalgarno,^d Marco Evangelisti,^{*c} Euan K. Brechin^{*d} and Constantinos J. Milios^{*a}

^a Department of Chemistry, University of Crete, Voutes 71003, Herakleion, Greece. Tel: +30-2810-545099; E-mail: kamil@uoc.gr

^b EaStCHEM School of Chemistry, The University of Edinburgh, David Brewster Road, Edinburgh, Scotland, EH9 3FJ, UK.

^c Instituto de Nanociencia y Materiales de Aragón (INMA), CSIC – Universidad de Zaragoza, 50009 Zaragoza, Spain.

^d Institute of Chemical Sciences, Heriot-Watt University, Riccarton, Edinburgh, Scotland, EH14 4AS, UK.

Electronic Supplementary Information (ESI) contains:

PXRD patterns (Fig. S1)	p. S2
EDS spectra (Fig. S2)	p. S3
SHAPE calculations (Table S1)	p. S4
<i>M</i> versus applied magnetic field for 2 collected for <i>T</i> = 2-10 K up to 7 T magnetic field.	p. S6

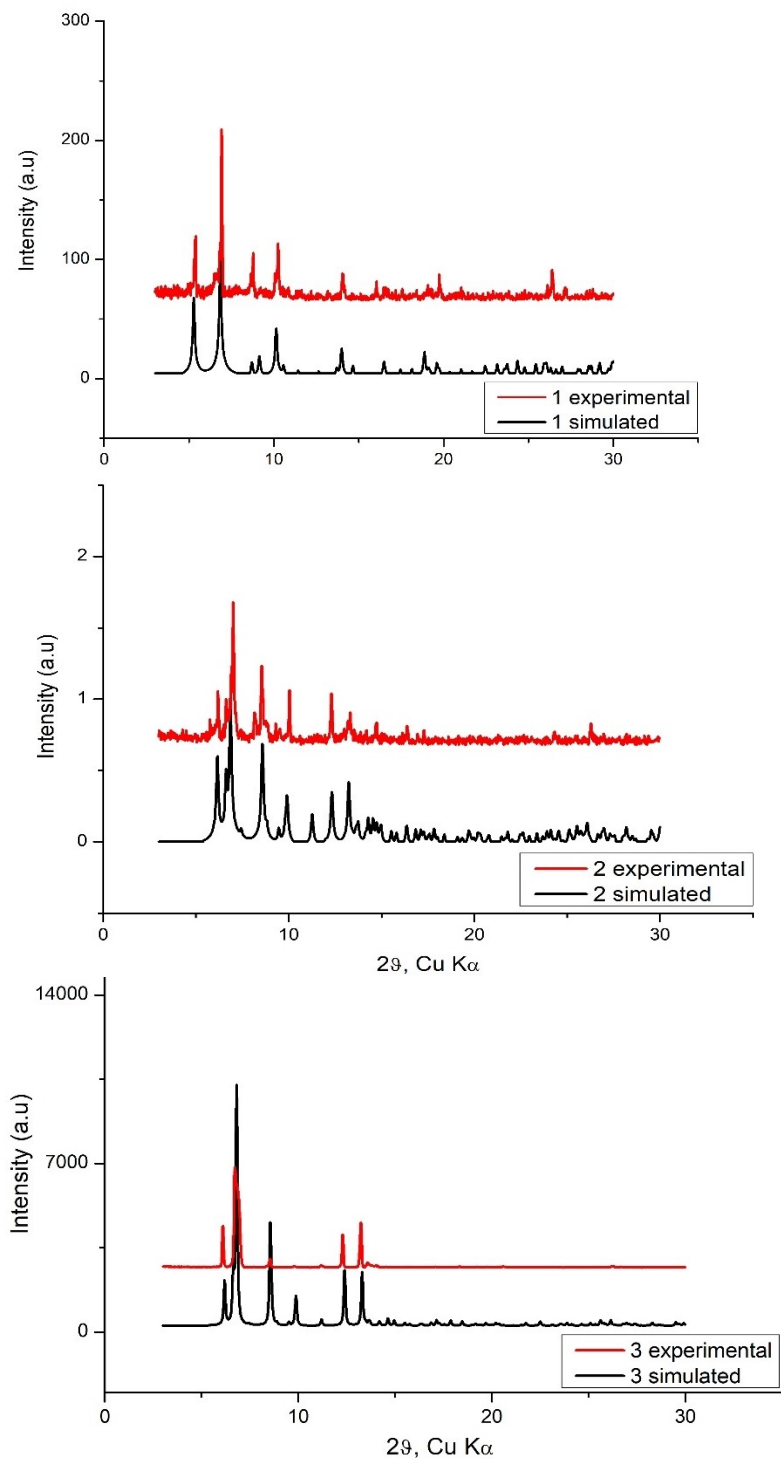


Fig S1. Powder XRD pattern comparison for **1 - 3** (top-to-bottom) and their simulated PXRD patterns. The differences in the peaks' intensity are due to solvent loss and preferred crystal orientation.

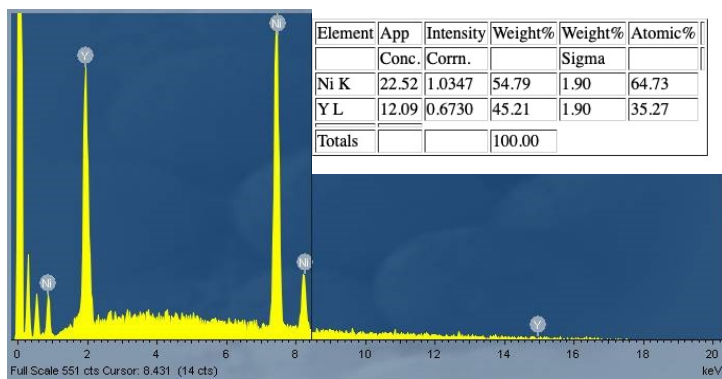
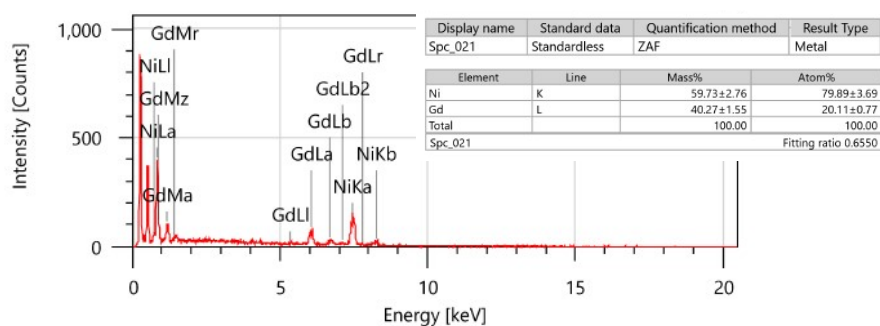
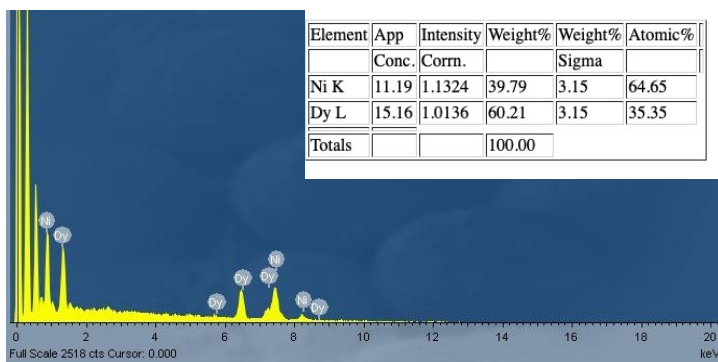


Fig S2. The EDS spectra for **1 – 3** (top to bottom).

Table S1. SHAPE calculations for Dy^{III}, Gd^{III} and Y^{III} centres in **1**, **2** and **3**, respectively.

Complex **1**: Dy1, Dy1'

Octagon	27.145
Heptagonal pyramid	20.834
Hexagonal bipyramid	15.876
Cube	9.766
Square antiprism	<u>0.584</u>
Triangular dodecahedron	2.869
Johnson gyrobifastigium J26	16.002
Johnson elongated triangular bipyramid	26.867
Biaugmented trigonal prism J50	3.091

Complex **1**: Dy2, Dy2'

Octagon	26.962
Heptagonal pyramid	20.747
Hexagonal bipyramid	15.795
Cube	9.766
Square antiprism	<u>0.626</u>
Triangular dodecahedron	2.713
Johnson gyrobifastigium J26	15.926
Johnson elongated triangular bipyramid	26.471
Biaugmented trigonal prism J50	3.205

Complex **3**: Y1, Y1'

Octagon	27.586
Heptagonal pyramid	20.202
Hexagonal bipyramid	15.864
Cube	9.598
Square antiprism	<u>0.735</u>
Triangular dodecahedron	2.764
Johnson gyrobifastigium J26	16.193
Johnson elongated triangular bipyramid	26.309
Biaugmented trigonal prism J50	3.337

Complex **3**: Y2, Y2'

Octagon	27.152
Heptagonal pyramid	20.077
Hexagonal bipyramid	15.870
Cube	9.880
Square antiprism	<u>0.729</u>
Triangular dodecahedron	2.916
Johnson gyrobifastigium J26	16.017
Johnson elongated triangular bipyramid	26.190
Biaugmented trigonal prism J50	3.350
Johnson elongated triangular bipyramid	26.194
Biaugmented trigonal prism J50	3.311

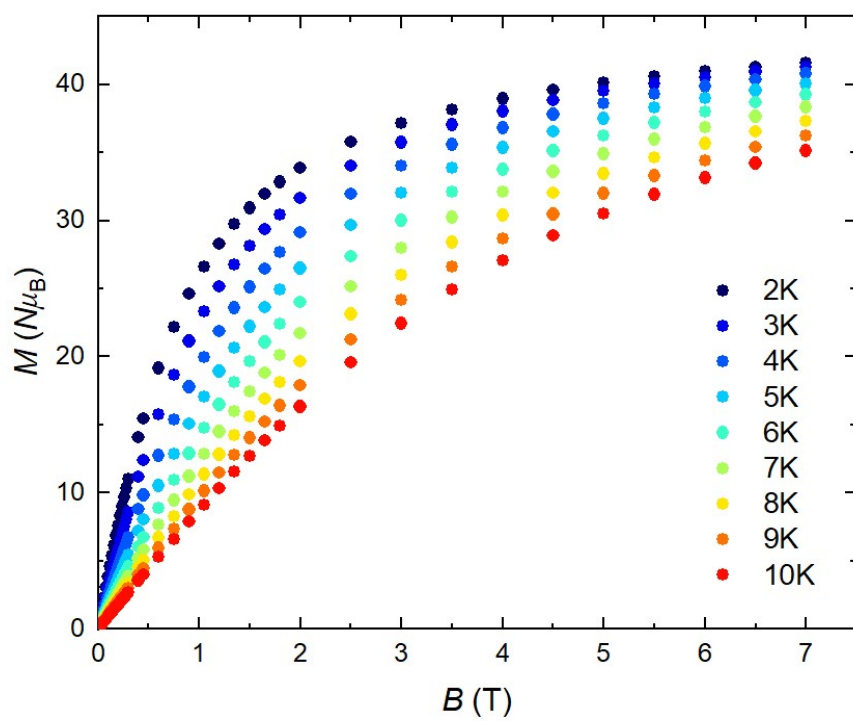


Fig S3. Isothermal molar magnetization M versus applied magnetic field, for **2**, collected for $T = 2$ -10 K, up to 7.0 T.