

Supporting Information

Solvothermal synthesis of enneanuclear $[\text{Cu}^{\text{II}}_7\text{Ln}^{\text{III}}_2]$
clusters

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Table S1. Crystallographic data for complex **1**.

	1·2MeCN
Formula	C ₁₀₂ H ₁₀₄ Cu ₇ Gd ₂ N ₈ O ₂₆
<i>M</i> _w	2617.21
Crystal System	Triclinic
Space group	P-1
<i>a</i> /Å	11.991 (3)
<i>b</i> / Å	14.520 (4)
<i>c</i> /Å	16.537 (4)
<i>α</i> /°	68.40 (2)
<i>β</i> /°	69.42 (2)
<i>γ</i> /°	84.05 (2)
<i>V</i> /Å ³	2505.1 (12)
<i>Z</i>	1
<i>T</i> /K	170
<i>λ</i> /Å	0.71073
<i>D</i> _c /g cm ⁻³	1.735
<i>μ</i> (Mo-Kα)/ mm ⁻¹	2.84
Meas./indep. (<i>R</i> _{int}) refl.	25865 / 12167 (0.054)
Obs. refl. [<i>I</i> > 2σ(<i>I</i>)]	8542
<i>wR</i> ²	0.105
<i>R</i> ¹	0.045
Goodness of fit on <i>F</i> ²	1.00
Δρ _{max,min} / eÅ ⁻³	1.03, -1.03

Table S2. Selected bond distances (°) and angles (Å) for complex **1**.

Gd—O14C	2.286 (3)	Cu1—O14A ⁱ	1.956 (3)
Gd—O15B	2.317 (3)	Cu1—O14A	1.956 (3)
Gd—O14A ⁱ	2.322 (3)	Cu1—O15A ⁱ	1.987 (3)
Gd—O15A	2.422 (3)	Cu1—O15A	1.987 (3)
Gd—O3	2.432 (4)	Cu1—O1	2.399 (3)
Gd—O2 ⁱ	2.436 (3)	Cu1—O1 ⁱ	2.399 (3)
Gd—O4	2.454 (4)	Cu2—O2A	1.887 (3)
Gd—O14B	2.541 (3)	Cu2—N1A	1.913 (4)
Cu3—O14B	1.976 (3)	Cu2—O14B	1.956 (3)
Cu3—O1	1.994 (3)	Cu2—O15A	1.984 (3)
Cu4—O2C	1.885 (3)	Cu3—O2B	1.895 (3)
Cu4—O14C	1.920 (3)	Cu3—N1N	1.924 (4)
Cu4—N1C	1.927 (4)	Cu4—O15B	1.946 (3)
O15A—Gd—O2 ⁱ	75.45 (10)	O14C—Gd—O14B	137.27 (11)
O3—Gd—O2 ⁱ	112.10 (13)	O15B—Gd—O14B	74.89 (10)
O14C—Gd—O4	83.48 (13)	O14A ⁱ —Gd—O14B	73.06 (10)
O15B—Gd—O4	101.32 (15)	O15A—Gd—O14B	65.06 (10)
O14A ⁱ —Gd—O4	159.24 (14)	O3—Gd—O14B	71.71 (12)
O15A—Gd—O4	104.81 (13)	O2 ⁱ —Gd—O14B	138.58 (10)
O3—Gd—O4	52.57 (14)	O4—Gd—O14B	123.77 (12)
O2 ⁱ —Gd—O4	77.10 (14)	O14A ⁱ —Cu1—O14A	180.0
O15A—Cu1—O1	87.17 (12)	O14A ⁱ —Cu1—O15A ⁱ	93.30 (12)
O14A ⁱ —Cu1—O1 ⁱ	99.81 (12)	O14A—Cu1—O15A ⁱ	86.70 (12)
O14A—Cu1—O1 ⁱ	80.19 (12)	O14A ⁱ —Cu1—O15A	86.70 (12)
O15A ⁱ —Cu1—O1 ⁱ	87.17 (12)	O14A—Cu1—O15A	93.30 (12)
O15A—Cu1—O1 ⁱ	92.83 (12)	O15A ⁱ —Cu1—O15A	180.0
O1—Cu1—O1 ⁱ	180.0	O14A ⁱ —Cu1—O1	80.19 (12)
O15A ⁱ —Cu1—O1	92.83 (12)	O14A—Cu1—O1	99.81 (12)
O2A—Cu2—N1A	94.38 (15)	O2B—Cu3—N1N	93.76 (16)
O2A—Cu2—O14B	95.50 (13)	O2B—Cu3—O14B	176.22 (13)
N1A—Cu2—O14B	170.10 (15)	N1N—Cu3—O14B	84.26 (15)
O2A—Cu2—O15A	177.19 (13)	O2B—Cu3—O1	92.04 (13)
N1A—Cu2—O15A	84.76 (14)	N1N—Cu3—O1	168.93 (15)
O14B—Cu2—O15A	85.34 (13)	O14B—Cu3—O1	90.44 (12)

O2C—Cu4—O15B	99.09 (14)	O2C—Cu4—O14C	176.81 (15)
O14C—Cu4—O15B	82.41 (13)	O2C—Cu4—N1C	93.17 (16)
N1C—Cu4—O15B	163.58 (16)	O14C—Cu4—N1C	85.91 (15)

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x, -y+1, -z+1$; (iii) $-x, -y, -z+1$.

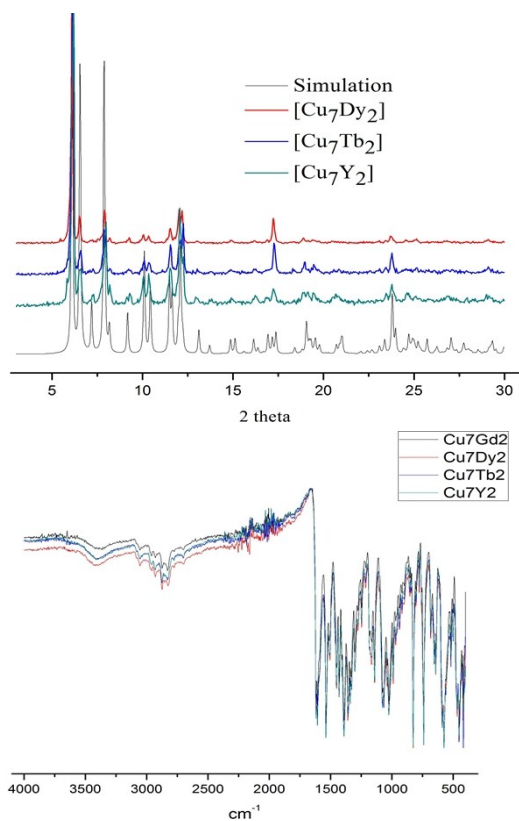


Fig. S1 Powder XRD diagrams' comparison between **2**, **3** and **4**, with the simulated PXRD diagram of the Gd analogue, **1** (top); IR spectra comparison for **1-4** (bottom).

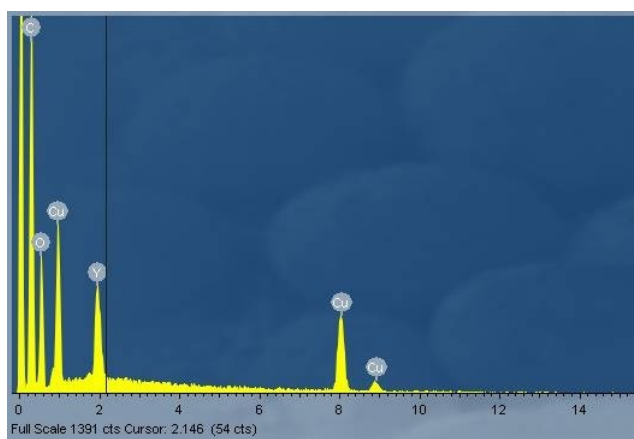


Fig.S2 Representative Energy Dispersive X-ray Spectroscopy analysis for the $[\text{Cu}^{\text{II}}_7\text{Y}^{\text{III}}_2]$ analogue, **4**.