

## **Electronic Supplementary Information (ESI) for**

# **Crystal structures and magnetic properties of two series of phenoxo-*O* bridged dinuclear Ln<sub>2</sub> (Ln = Gd, Tb, Dy) complexes**

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**Table S1** Basic crystallographic data for compounds **1a–c** and **2a–c**

	<b>1a</b>	<b>1b</b>	<b>1c</b>	<b>2a</b>	<b>2b</b>	<b>2c</b>
Formula	C <sub>66</sub> H <sub>76</sub> Gd <sub>2</sub> N <sub>2</sub> O <sub>18</sub>	C <sub>66</sub> H <sub>76</sub> Tb <sub>2</sub> N <sub>2</sub> O <sub>18</sub>	C <sub>66</sub> H <sub>76</sub> Dy <sub>2</sub> N <sub>2</sub> O <sub>18</sub>	C <sub>64</sub> H <sub>58</sub> Gd <sub>2</sub> N <sub>4</sub> O <sub>12</sub>	C <sub>64</sub> H <sub>58</sub> Tb <sub>2</sub> N <sub>4</sub> O <sub>12</sub>	C <sub>64</sub> H <sub>58</sub> Dy <sub>2</sub> N <sub>4</sub> O <sub>12</sub>
<i>M</i> (g·mol <sup>-1</sup> )	1499.79	1503.12	1510.28	1389.64	1392.98	1400.14
Crystal system	Triclinic	Triclinic	Triclinic	Monoclinic	Monoclinic	Monoclinic
Space group	<i>P</i> $\bar{1}$	<i>P</i> $\bar{1}$	<i>P</i> $\bar{1}$	<i>P</i> 2 <sub>1</sub> / <i>c</i>	<i>P</i> 2 <sub>1</sub> / <i>c</i>	<i>P</i> 2 <sub>1</sub> / <i>c</i>
<i>λ</i> (Å)	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073
<i>a</i> (Å)	10.9275(4)	10.8918(2)	10.8879(2)	11.2606(13)	11.2720(3)	11.2623(2)
<i>b</i> (Å)	12.2795(4)	12.2785(2)	12.2929(2)	15.9046(15)	15.8900(3)	15.7686(3)
<i>c</i> (Å)	13.7315(5)	13.6668(3)	13.6009(3)	15.5822(17)	15.5373(4)	15.5235(3)
<i>α</i> (°)	64.929(4)	65.133(2)	65.334(2)	90	90.00	90
<i>β</i> (°)	78.551(3)	78.645(2)	78.453(2)	96.903(5)	96.596(2)	96.256(2)
<i>γ</i> (°)	75.154(3)	75.204(2)	74.994(2)	90	90.00	90
<i>V</i> (Å <sup>3</sup> )	1604.71(11)	1594.92(6)	1589.06(6)	2770.5(5)	2764.50(12)	2740.41(9)
<i>Z</i>	1	1	1	2	2	2
<i>T</i> (K)	130(2)	130(2)	130(2)	150(2)	150(2)	130(2)
<i>ρ</i> <sub>calcd</sub> (g·cm <sup>-3</sup> )	1.552	1.565	1.578	1.666	1.673	1.697
<i>μ</i> (mm <sup>-1</sup> )	2.121	2.272	2.406	2.443	2.607	2.776
Data/restraints/ parameters	5631/0/402	5605/0/402	5579/0/401	5677/0/373	4868/0/373	4832/0/373
<i>R</i> <sub>int</sub>	0.0238	0.0198	0.0171	0.0757	0.0332	0.0277
<i>R</i> <sub>1</sub> <sup>a</sup> [ <i>I</i> > 2σ( <i>I</i> )] / <i>R</i> <sub>1</sub> (all)	0.0205/ 0.0241	0.0177/ 0.0201	0.0166/ 0.0183	0.0338/ 0.0511	0.0274/ 0.0428	0.0212/ 0.0273
<i>wR</i> <sub>2</sub> <sup>b</sup> [ <i>I</i> > 2σ( <i>I</i> )] / <i>wR</i> <sub>2</sub> (all)	0.0475/ 0.0481	0.0439/ 0.0443	0.0418/ 0.0421	0.0592/ 0.0632	0.0627/ 0.0671	0.0514/ 0.0525
Goodness-of-fit	1.025	1.105	1.079	1.084	1.030	1.037

**Table S2.** Parameters of one-component Debye model for Dy<sup>III</sup> complex **2c** derived according to eq.2 in the main text.

T/K	$\chi_s/(10^{-6} \text{ m}^3\text{mol}^{-1})$	$\chi_T/(10^{-6} \text{ m}^3\text{mol}^{-1})$	$\alpha$	$\tau/(10^{-3} \text{ s})$
1.90	13.95	219.83	0.348	1.373
2.15	0.29	195.90	0.434	1.089
2.41	11.11	167.78	0.394	1.141
2.66	11.90	150.05	0.398	1.041
2.91	3.63	135.50	0.455	0.751
3.17	4.52	121.88	0.450	0.597
3.42	8.28	110.83	0.461	0.474
3.67	2.88	99.76	0.431	0.280
3.92	4.76	92.58	0.457	0.184