Supporting Information

Dinuclear Lanthanide(III) Clusters Incorporated a Polydentate Schiff Base Ligand with Dy₂ Displaying Single-Molecule Magnet Behaviour

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Table S1 Selected bond lengths (Å) and angles (°) for compounds 1-3

| 1 | | 2 | | 3 | |
|---------------------|------------|---------------------|------------|-------------------|------------|
| N(1)-Gd(1) | 2.510(4) | N(1)-Tb(1) | 2.496(4) | Dy(1)-O(5) | 2.2300(19) |
| N(2)-Gd(1) | 2.780(4) | N(2)-Tb(1) | 2.769(4) | Dy(1)-O(1) | 2.2427(17) |
| Gd(1)-N(4)#1 | 2.523(4) | N(3) -Tb(1)#1 | 2.764(4) | Dy(1)-O(3)#1 | 2.3220(19) |
| N(4)-Gd(1)#1 | 2.522(4) | N(4)-Tb(1)#1 | 2.515(4) | Dy(1)-O(3) | 2.3296(17) |
| O(3)-Gd(1)#1 | 2.380(3) | O(1)-Tb(1) | 2.262(3) | Dy(1)-N(1) | 2.494(2) |
| O(3)-Gd(1) | 2.368(3) | O(3)-Tb(1) | 2.353(3) | Dy(1)-N(4) | 2.498(2) |
| O(5)-Gd(1)#1 | 2.270(3) | O(3)-Tb(1)#1 | 2.361(3) | Dy(1)-N(3) | 2.725(2) |
| Gd(1)-O(5)#1 | 2.270(3) | O(5)-Tb(1)#1 | 2.250(4) | Dy(1)-N(2)#1 | 2.752(2) |
| O(5)#1-Gd(1)-O(1) | 131.53(12) | O(5)#1-Tb(1)-O(1) | 131.79(13) | O(5)-Dy(1)-O(1) | 134.20(7) |
| O(5)#1-Gd(1)-O(3) | 142.31(11) | O(5)#1-Tb(1)-O(3) | 142.15(12) | O(5)-Dy(1)-O(3)#1 | 141.41(7) |
| O(1)-Gd(1)-N(1) | 71.06(13) | O(1)-Tb(1)-O(3) | 83.66(12) | O(5)-Dy(1)-N(1) | 74.77(7) |
| O(3)-Gd(1)-N(4)#1 | 142.66(12) | O(5)#1-Tb(1)-N(1) | 73.90(14) | O(1)-Dy(1)-N(1) | 71.08(7) |
| O(3)#1-Gd(1)-N(4)#1 | 112.94(9) | O(1)-Tb(1)-N(1) | 71.23(14) | O(3)-Dy(1)-N(4) | 115.53(7) |
| O(1)-Gd(1)-N(2) | 112.87(12) | O(3)-Tb(1)-N(1) | 115.12(13) | N(1)-Dy(1)-N(4) | 83.47(7) |
| N(3)#1-Gd(1)-N(2) | 147.73(11) | O(1)-Tb(1)-N(4)#1 | 73.67(14) | O(5)-Dy(1)-N(3) | 110.90(7) |
| O(5)#1-Gd(1)-N(3)#1 | 112.16(12) | O(3)-Tb(1)-N(4)#1 | 142.67(13) | O(1)-Dy(1)-N(3) | 82.42(7) |
| O(1)-Gd(1)-N(3)#1 | 81.21(12) | O(5)#1-Tb(1)-N(3)#1 | 112.06(13) | O(3)-Dy(1)-N(2)#1 | 81.75(6) |
| O(3)-Gd(1)-N(3)#1 | 82.43(11) | O(1)-Tb(1)-N(3)#1 | 81.10(13) | N(1)-Dy(1)-N(2)#1 | 66.16(7) |
| O(3)#1-Gd(1)-N(3)#1 | 70.43(11) | O(1)-Tb(1)-N(2) | 112.66(13) | N(4)-Dy(1)-N(2)#1 | 143.18(7) |
| N(1)-Gd(1)-N(3)#1 | 144.73(12) | N(4)#1-Tb(1)-N(2) | 145.11(13) | N(3)-Dy(1)-N(2)#1 | 148.35(6) |

Symmetry transformations used to generate equivalent atoms: Gd, Tb: #1 -x,-y+1,-z+1; Dy: #1 -x,-y,-z.



Figure S1. The M vs. H plot of 3 collected at 2 K. Data were simulated using MAGPACK (solid line), see the main text for parameters.



Figure S2. $M \operatorname{vs} H/T$ plots for **2** at indicated temperatures.



Figure S3. Temperature dependence of in-phase (χ') and out-of-phase (χ'') (bottom) ac susceptibilities of **2** at 997 Hz in zero dc field and 3 Oe ac field.



Figure S4. Temperature dependence of in-phase (χ') and out-of-phase (χ'') (bottom) ac susceptibilities of **3** in zero dc field and 3 Oe ac field.



Figure S5. Out-of-phase ac susceptibility (χ'') collected on **3** at different temperature under a 800 Oe dc field for the frequencie of 997 Hz