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# Supporting Information

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## Pure Trinuclear 4f Single-Molecule Magnets: Synthesis, Structures, Magnetism and Ab Initio Investigation

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## Magnetic measurements

Magnetization data down to 0.5 K were collected with the same magnetometer equipped with a self-built 3He cryostat (i-Quantum).

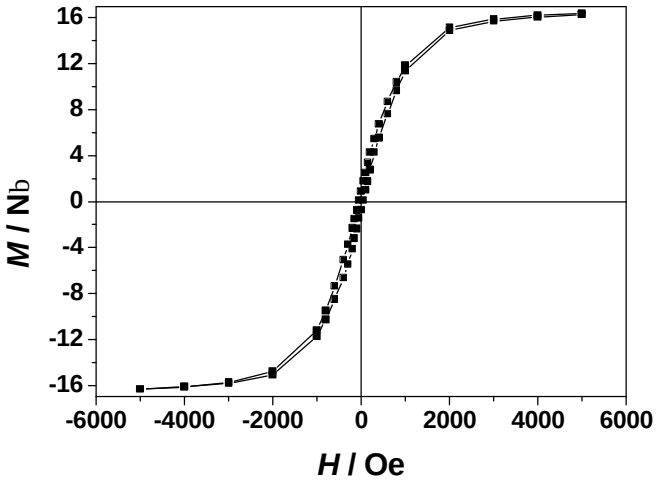


***Figure S1.*** Magnetic hysteresis loop at 0.5 K for **1**.

**Table S1.** Relaxation fitting parameters from Least-Squares Fitting of $c(w)$ data

| $T$ (K) | $c_0$ $cm^3mol^{-1}$ | $c_1$ $cm^3mol^{-1}$ | $c_2$ $cm^3mol^{-1}$ | $a_1$ | $a_2$ | $t_1$ | $t_2$ |
|---|---|---|---|---|---|---|---|
| 4.6 | 10.91744 | 8.2174 | 0.61877 | 0.04877 | 0.61526 | 0.03617 | 0.0008 |
| 4.8 | 10.25163 | 7.72155 | 0.77444 | 0.03766 | 0.59269 | 0.03077 | 0.00061 |
| 5.0 | 9.67007 | 7.2537 | 0.8774 | 0.03235 | 0.57163 | 0.02575 | 0.00045 |
| 5.2 | 9.16557 | 6.82119 | 0.93922 | 0.03322 | 0.55223 | 0.02129 | 0.00032 |
| 5.4 | 8.72397 | 6.44986 | 0.9648 | 0.03442 | 0.53622 | 0.01745 | 0.00024 |
| 5.7 | 8.14801 | 5.96922 | 0.96269 | 0.0382 | 0.51627 | 0.01281 | 0.00015 |
| 6.0 | 7.59821 | 5.52957 | 1.06913 | 0.03417 | 0.48507 | 0.00917 | 0.0001 |