Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information:

The effect of additional methyl on the magnetic relaxation and toroidal moment of Dy_6 complex

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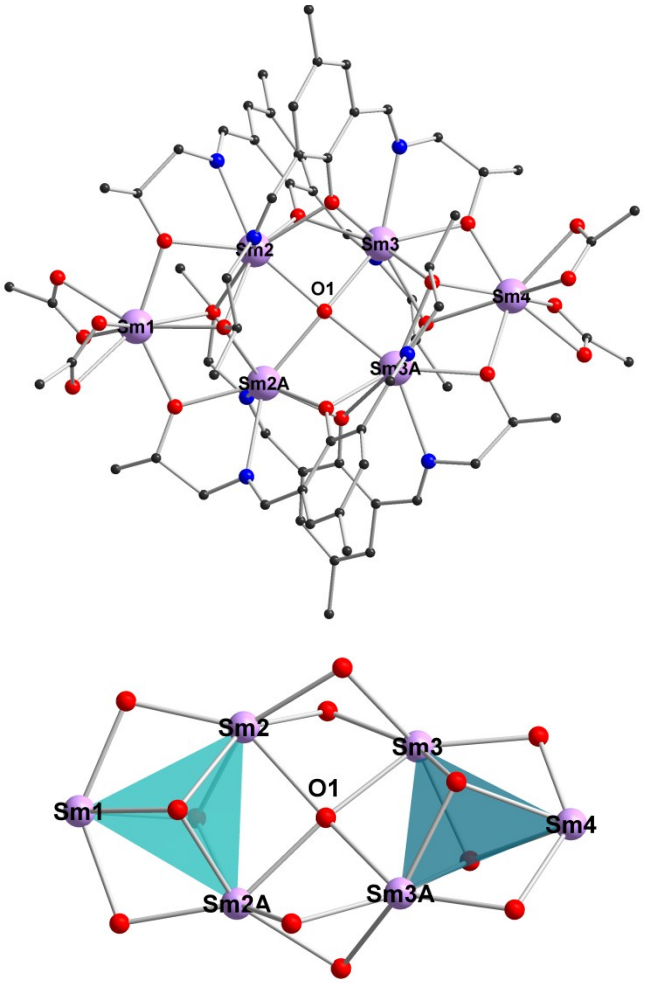

Fig. S1 Structure of 2 with hydrogen atoms omitted for clarity.

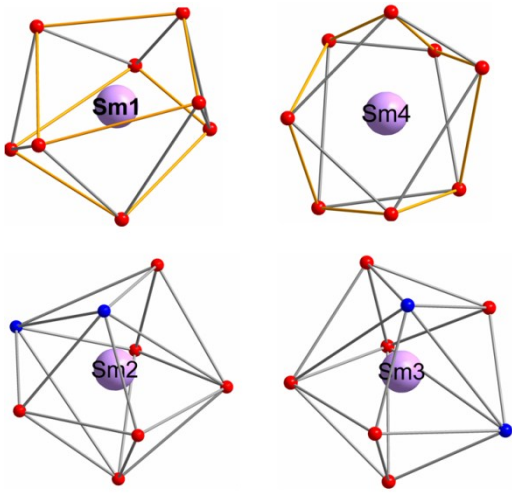

Fig. S2 Coordination polyhedra (distorted square antiprism for Sm1 and Sm4; distorted triangular dodecahedron for Sm2 and Sm3) for four Sm^{3+} ions in 2.

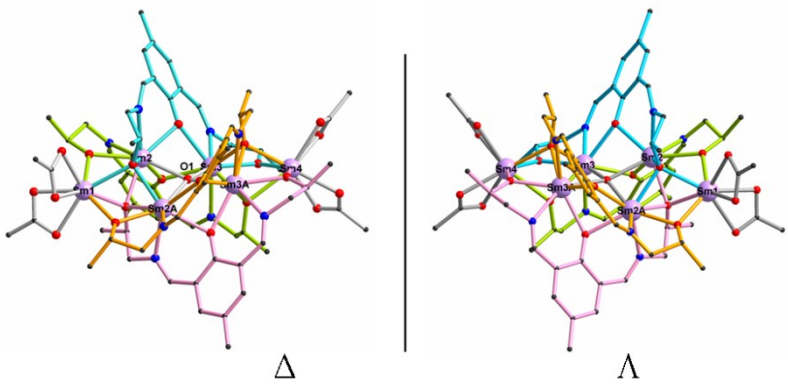

Fig. S3 Two stereoisomers of right- (Δ) and left-hand (Λ) configurations in 2.

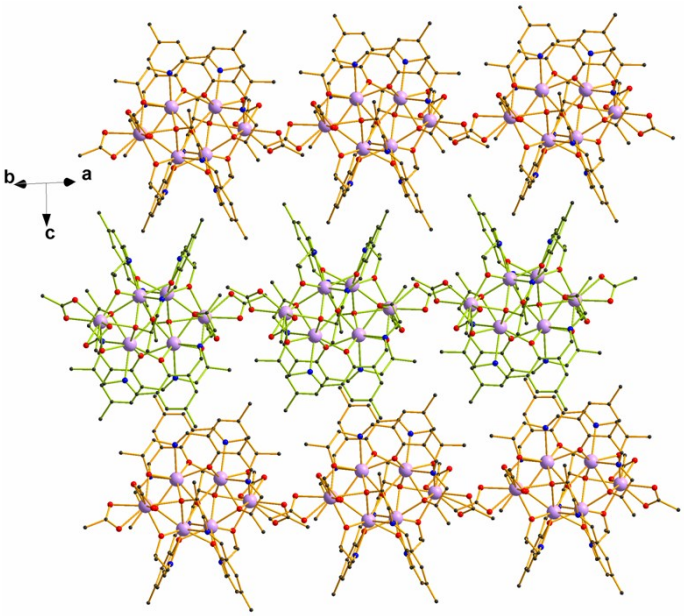

Fig. S4 Crystal packing of **2** showing the stereoisomers.

Table S1. The CShM values calculated by *SHAPE* 2.1 for compound **1** and Dy_6-2.

	Site	Coordination surrounding	Square antiprism	Triangular dodecahedron	Biaugmented trigonal prism
1	Dy1	6O2N	**1.590**	1.969	2.385
	Dy2	6O2N	2.015	**1.557**	2.515
	Dy3	6O2N	**1.608**	1.688	2.303
	Dy4	6O2N	1.687	**1.522**	2.329
	Dy5	8O	**3.330**	4.549	4.456
	Dy6	8O	**2.382**	4.480	4.006
Dy_6-2	Dy1	6O2N	**1.447**	1.695	2.106
	Dy2	6O2N	1.884	**1.664**	2.520
	Dy3	6O2N	**1.441**	1.820	2.123
	Dy4	6O2N	1.697	**1.696**	2.563
	Dy5	8O	**2.585**	3.420	3.365
	Dy6	9O	**CSAPR-9*, 2.034**	TCTPR-9*, 2.965	--

*CSAPR-9: Spherical capped square antiprism;

*TCTPR-9: Spherical tricapped trigonal prism.

Table S2. The CShM values calculated by *SHAPE* 2.1 for compound **2**.

	Coordination surrounding	Square antiprism	Triangular dodecahedron	Biaugmented trigonal prism
Sm1	8O	**2.465**	4.547	4.484
Sm2	6O2N	2.008	**1.909**	2.819
Sm3	6O2N	2.219	**1.686**	2.626
Sm4	8O	**2.998**	4.370	4.987

Table S3. Minimal reorientation energies (cm^{-1}) calculated from Magellan program for complex **1**.

Site	Dy1	Dy2	Dy3	Dy4	Dy5	Dy6
Min. reorientation energy (cm^{-1})	619.2	791.7	598.7	605.0	768.0	587.3