Supporting Information for

Diacylhydrazone Assembled {Ln_{11}} Nanoclusters Featuring a "Double-Boats Conformation" Topology: Synthesis, Structures, and Magnetism

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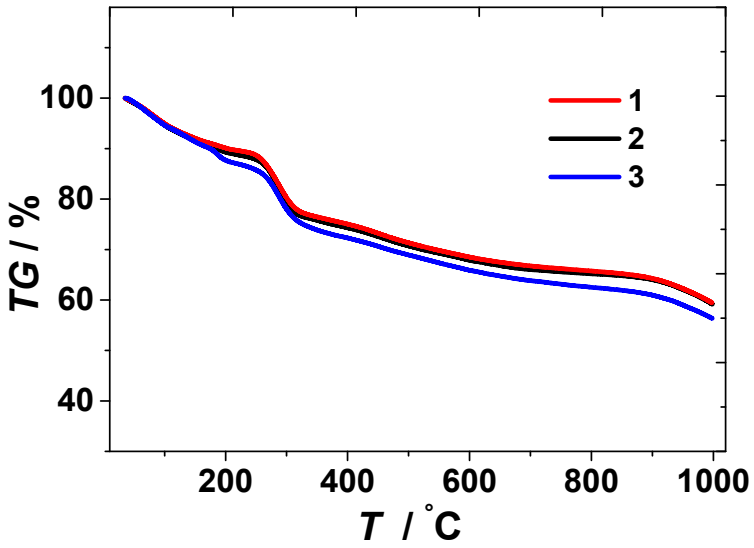


Fig. S1 The TG plots of **1-3.**

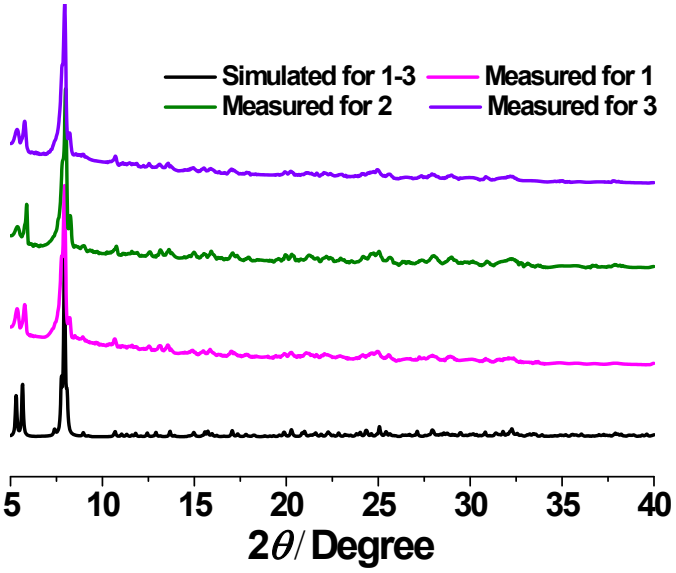
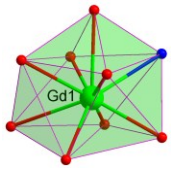
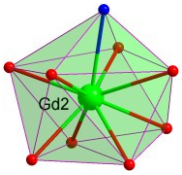
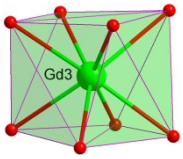
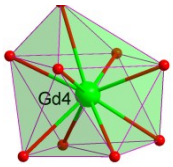
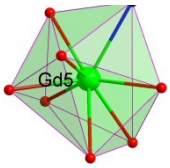
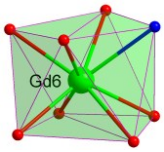


Fig. S2 The PXRD patterns of **1-3.**

Table S1 The coordination environments, geometries and donors for the Gd^{3+} ions in **1**.

Gd^{3+} ions	Coordination Environments	Coordination Geometries	Coordination Donors
Gd1		Nine-coordinated mono-capped square antiprism	O_{phenol}, O_{enol}, $N_{acylhydrazone}$, $O_{methoxyl}$, μ_3-$O_{hydroxyl}$, $O_{nitrate}$
Gd2		Nine-coordinated mono-capped square antiprism	O_{phenol}, O_{enol}, $N_{acylhydrazone}$, $O_{methanol}$, $O_{oxynitride}$, μ_3-$O_{hydroxyl}$
Gd3		Eight-coordinated square antiprism	O_{enol}, $O_{oxynitride}$, μ_3-$O_{hydroxyl}$
Gd4		Nine-coordinated mono-capped square antiprism	O_{enol}, $O_{oxynitride}$, $O_{methanol}$, $O_{nitrate}$, μ_3-$O_{hydroxyl}$, $O_{aqueous}$
Gd5		Eight-coordinated serious distorted bicapped triprism	O_{phenol}, O_{enol}, $N_{acylhydrazone}$, $O_{methanol}$, $O_{nitrate}$, μ_2-$O_{hydroxyl}$, μ_3-$O_{hydroxyl}$
Gd6		Eight-coordinated square antiprism	O_{phenol}, O_{enol}, $N_{acylhydrazone}$, $O_{methoxyl}$, $O_{methanol}$, μ_2-$O_{hydroxyl}$, μ_3-$O_{hydroxyl}$

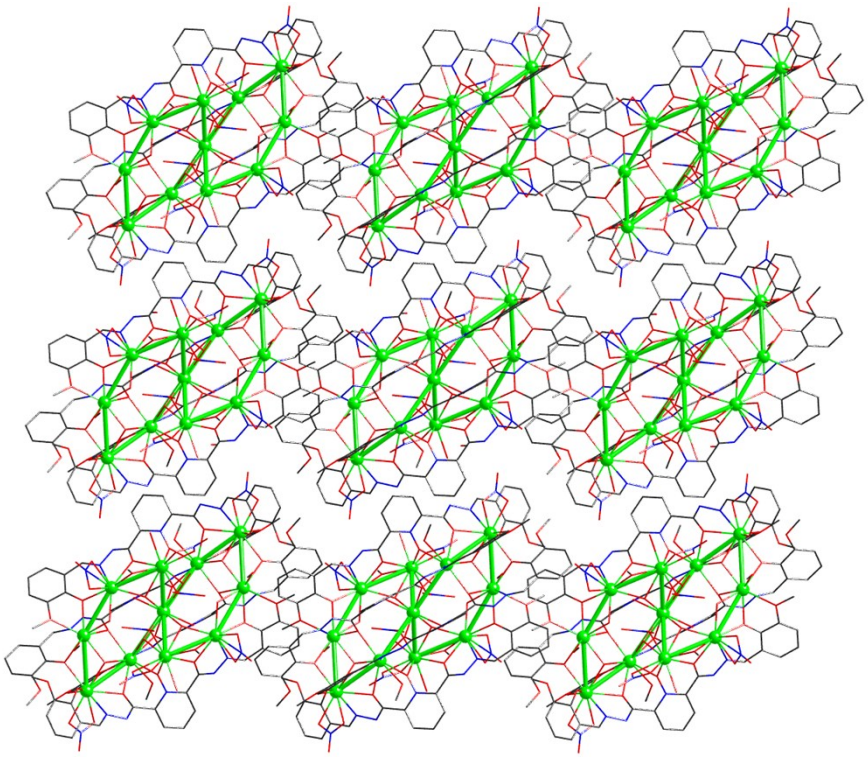


Fig. S3 Packing diagram of **1** viewed from *b*-axis direction.

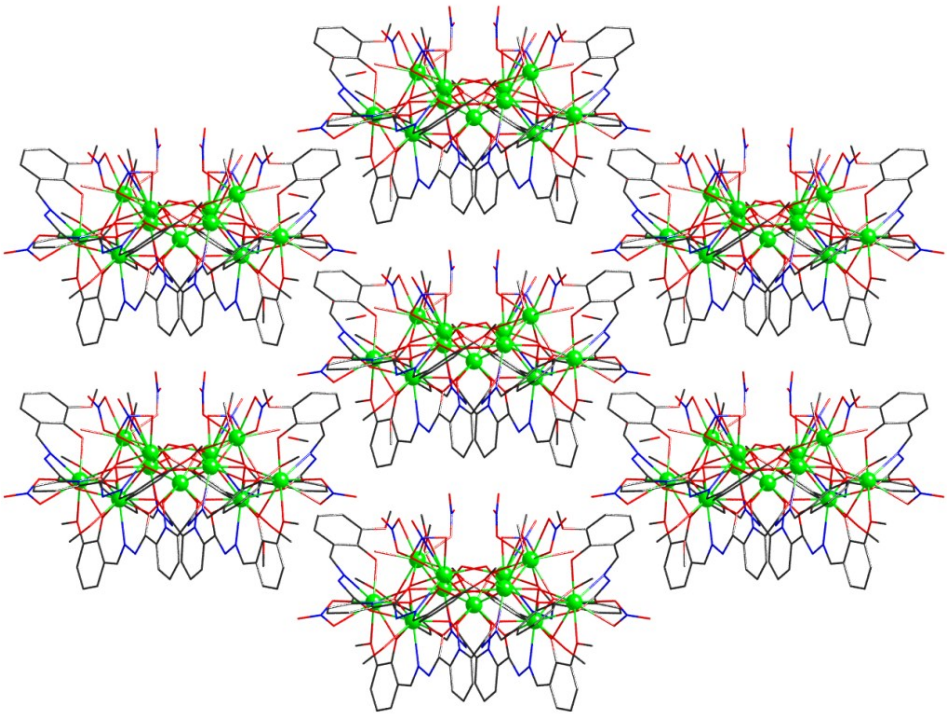


Fig. S4 Packing diagram of **1** viewed from *c*-axis direction.

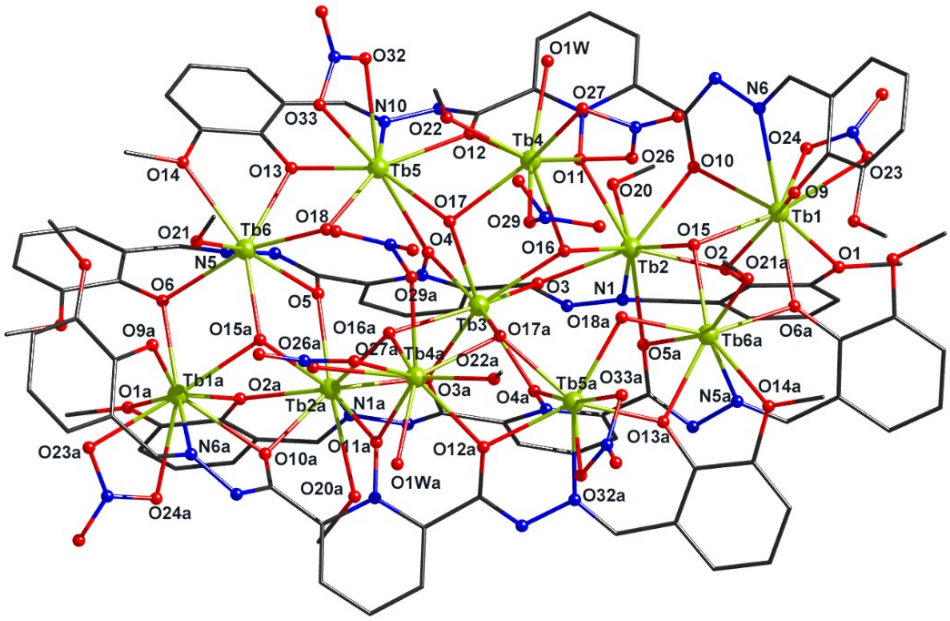


Fig. S5 The molecular structure of **2** (symmetry code: a, −x+1, y, −z+0.5). Color scheme: black for C, red for O, blue for N and lime for Tb.

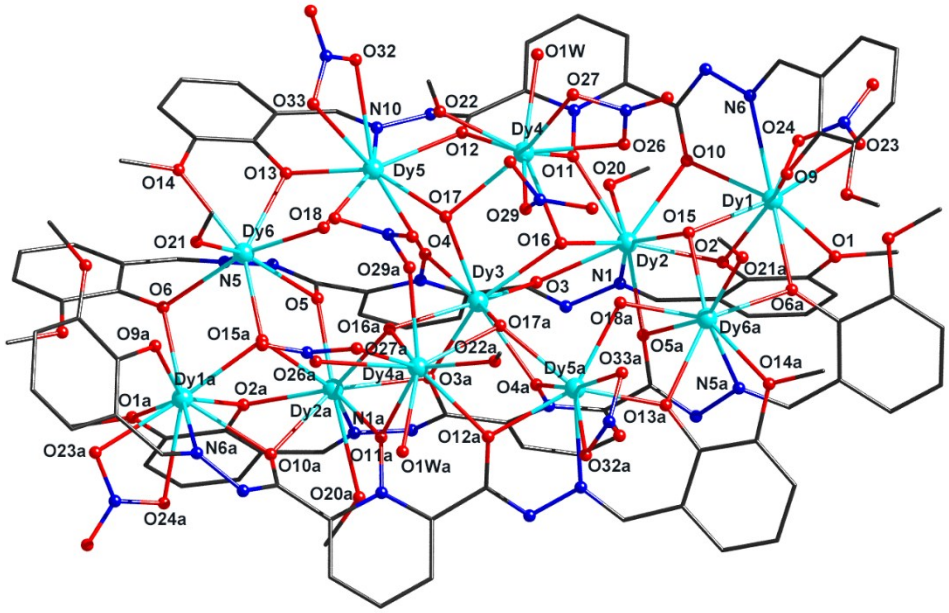


Fig. S6 The molecular structure of **3** (symmetry code: a, −x+1, y, −z+0.5). Color scheme: black for C, red for O, blue for N and turquoise for Dy.

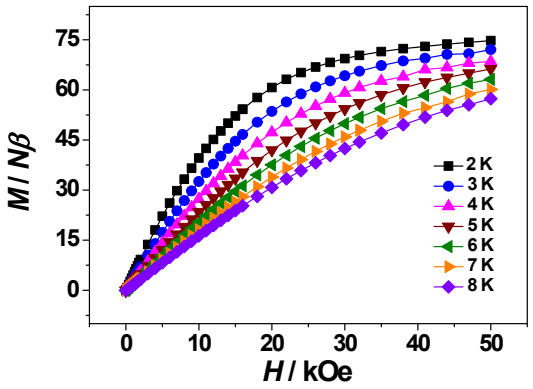


Fig. S7 Plots of *M*-*H* of **1** in the range of *T* = 2.0-8.0 K and *H* = 0-50 kOe.

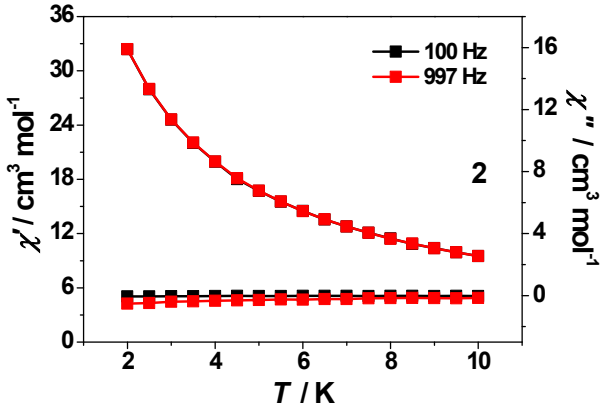


Fig. S8 Temperature-dependent ac susceptibility of **2** under a 2.5 Oe ac field and 0 Oe dc field.

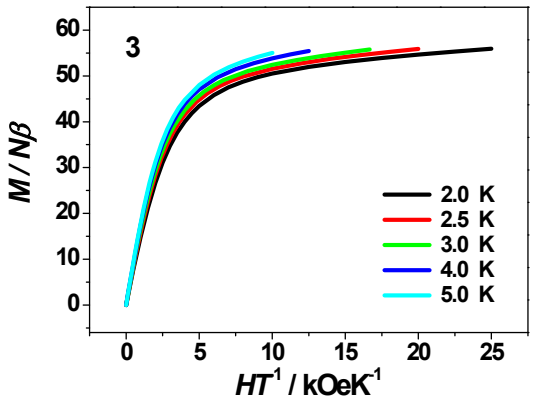


Fig. S9 Plots of *M*-*HT*$^{-1}$ of **3** at different temperature.

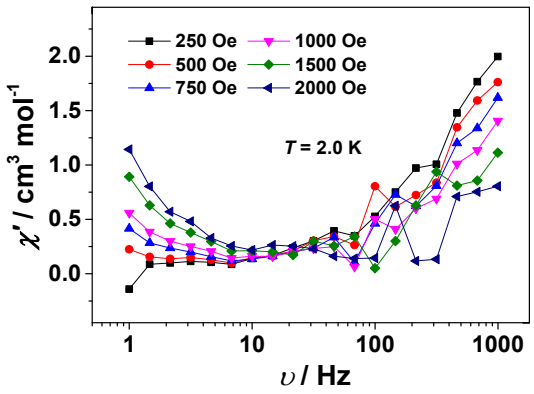


Fig. S10 Plots of χ''-v of **3** collected at 2.0 K under various dc fields.

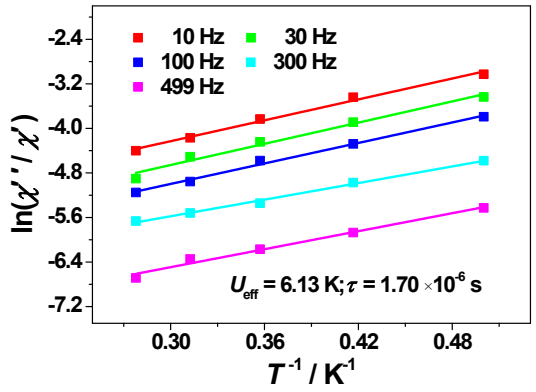


Fig. S11 Plots of ln(χ''/χ')-T^{-1} for **3**.

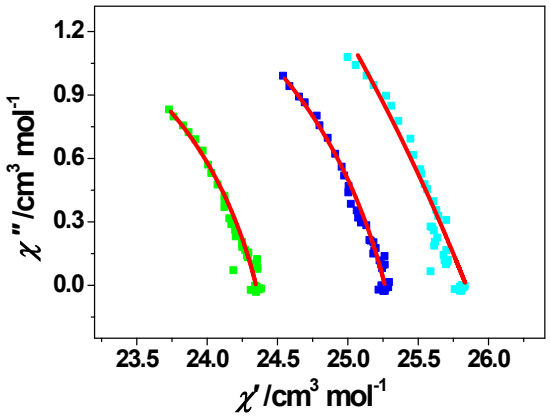


Fig. S12 Cole-Cole plots at 2.0-2.3 K for **3**. The solid lines are the best fits to the experimental data, obtained with the generalized Debye mode.

Table S2. Crystal data and structure refinement parameters for **1-3**.

Identification	**1**	**2**	**3**
Formula	$C_{101}H_{113}Gd_{11}N_{28}O_{73}$	$C_{101}H_{113}Tb_{11}N_{28}O_{73}$	$C_{101}H_{111}Dy_{11}N_{28}O_{72}$
Fw	4616.94	4635.30	4656.67
Temp./K	120.15	120.15	120.15
Crystal system	monoclinic	monoclinic	monoclinic
Space group	*C2/c*	*C2/c*	*C2/c*
a/Å	31.361(4)	31.3869(5)	31.3535(12)
b/Å	12.9403(15)	12.88765(16)	12.8876(5)
c/Å	33.405(4)	33.2931(4)	33.2676(6)
α/°	90.00	90.00	90.00
β/°	94.857(2)	94.6758(12)	94.675(3)
γ/°	90.00	90.00	90.00
V/Å^3	13508(3)	13422.4(3)	13397.7(7)
Z	4	4	4
D_c/g cm^{-3}	2.270	2.294	2.309
*m*μ/mm^{-1}	5.433	5.828	6.166
F(000)	8812.0	8856.0	8860.0
Reflns collected	52765	66443	65503
Unique reflns	11677	13156	13130
R_{int}	0.0682	0.0580	0.0509
GOF	1.133	1.070	1.190
R_1, wR_2 ($I > 2\sigma(I)$)	$R_1 = 0.0781$, $wR_2 = 0.1824$	$R_1 = 0.0538$ $wR_2 = 0.1277$	$R_1 = 0.0487$ $wR_2 = 0.1064$
R_1, wR_2 (all data)	$R_1 = 0.0917$ $wR_2 = 0.1910$	$R_1 = 0.0685$ $wR_2 = 0.1401$	$R_1 = 0.0562$ $wR_2 = 0.1117$

Table S3 Selected bond lengths (Å) and angles (°) for **1**.

Bond	Length (Å)	Bond	Length (Å)	Bond	Length (Å)
Gd1—O1	2.595 (10)	Gd3—O4^{i}	2.403 (9)	Gd5—O32	2.594 (16)
Gd1—O2	2.469 (9)	Gd3—O16	2.448 (8)	Gd5—O33	2.696 (18)
Gd1—O6^{i}	2.410 (9)	Gd3—O16^{i}	2.448 (8)	Gd5—N10	2.474 (13)
Gd1—O9	2.332 (10)	Gd3—O17	2.345 (8)	Gd5'—O12	2.404 (10)
Gd1—O10	2.490 (9)	Gd3—O17^{i}	2.345 (8)	Gd5'—O13	2.420 (11)
Gd1—O15	2.363 (8)	Gd4—O11	2.461 (9)	Gd5'—O17	2.397 (10)
Gd1—O23	2.474 (9)	Gd4—O12	2.420 (9)	Gd5'—O18	2.332 (10)
Gd1—O24	2.532 (11)	Gd4—O16	2.388 (8)	Gd5'—O22	2.533 (17)
Gd1—N6	2.525 (13)	Gd4—O17	2.406 (8)	Gd5'—O32	2.242 (15)
Gd2—O2	2.417 (9)	Gd4—O1W	2.427 (10)	Gd5'—O33	2.271 (17)
Gd2—O3	2.426 (8)	Gd4—H1WB	2.3811	Gd5'—N10	2.708 (14)
Gd2—O5^{i}	2.466 (8)	Gd4—O22	2.426 (13)	Gd6—O5	2.420 (9)
Gd2—O10	2.405 (9)	Gd4—O26	2.446 (10)	Gd6—O6	2.332 (10)
Gd2—O11	2.404 (10)	Gd4—O27	2.568 (16)	Gd6—O13	2.351 (10)
Gd2—O15	2.387 (9)	Gd4—O29	2.400 (9)	Gd6—O14	2.510 (10)
Gd2—O16	2.390 (8)	Gd5—O4	2.872 (10)	Gd6—O15^{i}	2.295 (9)
Gd2—O20	2.614 (9)	Gd5—O12	2.367 (10)	Gd6—O18	2.307 (10)
Gd2—N1	2.447 (16)	Gd5—O13	2.234 (11)	Gd6—O21	2.352 (10)
Gd3—O3^{i}	2.378 (8)	Gd5—O17	2.310 (10)	Gd6—N5	2.465 (13)
Gd3—O3	2.378 (8)	Gd5—O18	2.271 (10)		
Gd3—O4	2.404 (9)	Gd5—O22	2.928 (17)		
Bond Angle	**Angle(°)**	**Bond Angle**	**Angle(°)**	**Bond Angle**	**Angle(°)**
Gd2—O2—Gd1	98.8 (3)	Gd5—O13—Gd6	106.4 (4)	Gd3—O17—Gd5'	130.4 (4)
Gd3^{i}—O3—Gd2	113.5 (3)	Gd6—O13—Gd5'	108.2 (4)	Gd5—O17—Gd3^{i}	118.1 (4)
Gd3^{i}—O4—Gd5	97.9 (3)	Gd1—O15—Gd2	102.8 (3)	Gd5—O17—Gd4	107.2 (3)
Gd6—O5—Gd2^{i}	105.7 (3)	Gd6^{i}—O15—Gd1	108.7 (3)	Gd5'—O17—Gd4	100.7 (3)
Gd6—O6—Gd1^{i}	106.0 (4)	Gd6^{i}—O15—Gd2	112.6 (3)	Gd5—O18—Gd6	106.6 (4)
Gd2—O10—Gd1	98.6 (3)	Gd2—O16—Gd3^{i}	112.2 (3)	Gd6—O18—Gd5'	112.8 (4)
Gd2—O11—Gd4	111.4 (3)	Gd4—O16—Gd2	114.5 (3)	Gd4—O22—Gd5	89.8 (4)
Gd5—O12—Gd4	104.9 (4)	Gd4—O16—Gd3^{i}	105.5 (3)	Gd4—O22—Gd5'	96.5 (5)
Gd5'—O12—Gd4	100.2 (4)	Gd3—O17—Gd4	108.3 (3)		

Symmetry codes: (i) $-x+1, y, -z+1/2$.

Table S4 Selected bond lengths (Å) and angles (°) for **2**.

Bond	Length (Å)	Bond	Length (Å)	Bond	Length (Å)

Tb1—O1	2.589 (6)	Tb3—O3^{i}	2.375 (5)	Tb5—O32	2.592 (8)
Tb1—O2	2.464 (6)	Tb3—O4^{i}	2.396 (5)	Tb5—O33	2.684 (10)
Tb1—O6^{i}	2.391 (6)	Tb3—O4	2.396 (5)	Tb5—N10	2.445 (8)
Tb1—O9	2.312 (6)	Tb3—O16	2.443 (5)	Tb5'—O12	2.364 (6)
Tb1—O10	2.470 (6)	Tb3—O16^{i}	2.443 (5)	Tb5'—O13	2.406 (6)
Tb1—O15	2.335 (5)	Tb3—O17^{i}	2.333 (5)	Tb5'—O17	2.366 (6)
Tb1—O23	2.467 (6)	Tb3—O17	2.333 (5)	Tb5'—O18	2.344 (6)
Tb1—O24	2.524 (7)	Tb4—O11	2.436 (6)	Tb5'—O22	2.537 (10)
Tb1—N6	2.533 (8)	Tb4—O12	2.396 (6)	Tb5'—O32	2.265 (8)
Tb1—N11	2.899 (8)	Tb4—O16	2.371 (5)	Tb5'—O33	2.281 (10)
Tb2—O2	2.399 (6)	Tb4—O17	2.389 (5)	Tb5'—N10	2.689 (8)
Tb2—O3	2.423 (5)	Tb4—O1W	2.397 (7)	Tb5'—N14	2.661 (13)
Tb2—O5^{i}	2.434 (5)	Tb4—O22	2.398 (7)	Tb6—O5	2.422 (5)
Tb2—O10	2.400 (6)	Tb4—O26	2.429 (6)	Tb6—O6	2.324 (6)
Tb2—O11	2.422 (6)	Tb4—O27	2.581 (10)	Tb6—O13	2.358 (6)
Tb2—O15	2.370 (5)	Tb4—O29	2.377 (6)	Tb6—O14	2.534 (6)
Tb2—O16	2.361 (5)	Tb5—O4	2.850 (6)	Tb6—O15^{i}	2.292 (5)
Tb2—O20	2.633 (7)	Tb5—O12	2.359 (6)	Tb6—O18	2.304 (6)
Tb2—N1	2.359 (17)	Tb5—O13	2.183 (6)	Tb6—O21	2.363 (6)
Tb2—N1'	2.544 (17)	Tb5—O17	2.330 (6)	Tb6—N5	2.452 (8)
Tb3—O3	2.375 (5)	Tb5—O18	2.289 (6)		

Bond Angle	**Angle(°)**	**Bond Angle**	**Angle(°)**	**Bond Angle**	**Angle(°)**
Tb2—O2—Tb1	98.2 (2)	Tb5—O13—Tb6	106.7 (2)	Tb3—O17—Tb5'	130.0 (2)
Tb3—O3—Tb2	112.8 (2)	Tb6—O13—Tb5'	108.3 (2)	Tb5—O17—Tb3	117.6 (2)
Tb3—O4—Tb5	98.64 (18)	Tb1—O15—Tb2	102.7 (2)	Tb5—O17—Tb4	107.2 (2)
Tb6—O5—Tb2^{i}	104.7 (2)	Tb6^{i}—O15—Tb1	109.1 (2)	Tb5'—O17—Tb4	100.4 (2)
Tb6—O6—Tb1^{i}	106.1 (2)	Tb6^{i}—O15—Tb2	111.1 (2)	Tb5—O18—Tb6	105.0 (2)
Tb2—O10—Tb1	98.0 (2)	Tb2—O16—Tb3	112.6 (2)	Tb6—O18—Tb5'	112.4 (2)
Tb2—O11—Tb4	110.5 (2)	Tb2—O16—Tb4	115.1 (2)	Tb4—O22—Tb5'	95.4 (3)
Tb5—O12—Tb4	106.0 (2)	Tb4—O16—Tb3	105.53 (19)		
Tb5'—O12—Tb4	100.2 (2)	Tb3—O17—Tb4	108.5 (2)		

Symmetry codes: (i) $-x+1, y, -z+1/2$.

Table S5 Selected bond lengths (Å) and angles (°) for **3**.

Bond	**Length (Å)**	**Bond**	**Length (Å)**	**Bond**	**Length (Å)**
Dy1—O1	2.584 (7)	Dy3—O4	2.385 (6)	Dy5—O33	2.690 (11)
Dy1—O2	2.447 (6)	Dy3—O4^{i}	2.385 (6)	Dy5—N10	2.431 (8)
Dy1—O6^{i}	2.391 (6)	Dy3—O16^{i}	2.433 (5)	Dy5'—O12	2.347 (6)

Dy1—O9	2.285 (7)	Dy3—O16	2.433 (5)	Dy5'—O13	2.389 (7)
Dy1—O10	2.463 (7)	Dy3—O17^{i}	2.323 (6)	Dy5'—O17	2.365 (6)
Dy1—O15	2.329 (6)	Dy3—O17	2.323 (6)	Dy5'—O18	2.324 (6)
Dy1—O23	2.452 (7)	Dy4—O11	2.443 (7)	Dy5'—O22	2.553 (12)
Dy1—O24	2.519 (7)	Dy4—O12	2.399 (6)	Dy5'—O32	2.253 (9)
Dy1—N6	2.520 (9)	Dy4—O16	2.371 (6)	Dy5'—O33	2.270 (11)
Dy1—N11	2.887 (8)	Dy4—O17	2.378 (6)	Dy5'—N10	2.670 (8)
Dy2—O2	2.399 (6)	Dy4—O1W	2.391 (7)	Dy5'—N14	2.676 (15)
Dy2—O3	2.410 (6)	Dy4—O22	2.368 (9)	Dy6—O5	2.419 (6)
Dy2—O5^{i}	2.401 (6)	Dy4—O26	2.418 (7)	Dy6—O6	2.307 (6)
Dy2—O10	2.387 (6)	Dy4—O27	2.577 (11)	Dy6—O13	2.340 (6)
Dy2—O11	2.399 (7)	Dy4—O29	2.372 (7)	Dy6—O14	2.522 (7)
Dy2—O15	2.339 (6)	Dy5—O4	2.798 (6)	Dy6—O15^{i}	2.280 (6)
Dy2—O16	2.340 (6)	Dy5—O12	2.334 (6)	Dy6—O18	2.283 (6)
Dy2—O20	2.635 (8)	Dy5—O13	2.185 (7)	Dy6—O21	2.345 (6)
Dy2—N1	2.417 (11)	Dy5—O17	2.317 (6)	Dy6—N5	2.435 (8)
Dy3—O3	2.363 (6)	Dy5—O18	2.271 (6)		
Dy3—O3^{i}	2.363 (6)	Dy5—O32	2.598 (9)		

Bond Angle	**Angle(°)**	**Bond Angle**	**Angle(°)**	**Bond Angle**	**Angle(°)**
Dy2—O2—Dy1	97.9 (2)	Dy5—O13—Dy6	106.6 (3)	Dy3—O17—Dy5'	130.0 (3)
Dy3—O3—Dy2	112.7 (2)	Dy6—O13—Dy5'	108.5 (2)	Dy5—O17—Dy3	117.3 (2)
Dy3—O4—Dy5	99.44 (19)	Dy1—O15—Dy2	103.0 (2)	Dy5—O17—Dy4	107.0 (2)
Dy2^{i}—O5—Dy6	104.9 (2)	Dy6^{i}—O15—Dy1	108.7 (2)	Dy5'—O17—Dy4	100.2 (2)
Dy6—O6—Dy1^{i}	105.7 (2)	Dy6^{i}—O15—Dy2	111.7 (2)	Dy5—O18—Dy6	105.6 (2)
Dy2—O10—Dy1	97.7 (2)	Dy2—O16—Dy3	112.7 (2)	Dy6—O18—Dy5'	112.8 (3)
Dy2—O11—Dy4	110.3 (2)	Dy2—O16—Dy4	115.0 (2)	Dy2—O20—H20	119.4
Dy5—O12—Dy4	105.7 (2)	Dy4—O16—Dy3	105.1 (2)	Dy4—O22—Dy5'	95.3 (3)
Dy5'—O12—Dy4	100.1 (2)	Dy3—O17—Dy4	108.4 (2)		

Symmetry codes: (i) $-x+1, y, -z+1/2$.