

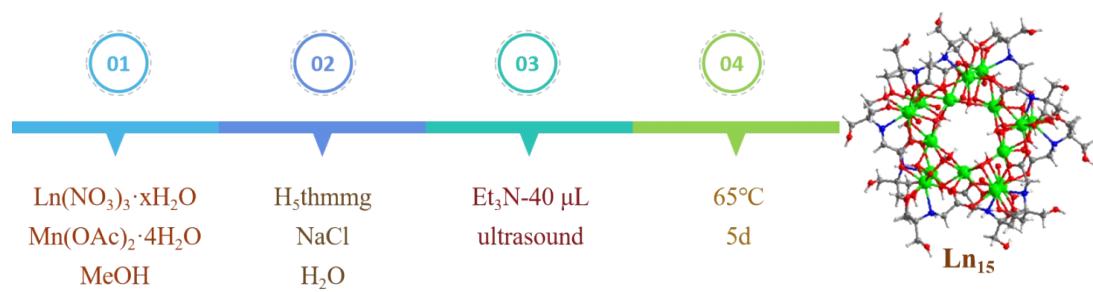
**Electronic Supplementary Information (ESI)**

**The pentagram-typed  $\text{Ln}_{15}$  ( $\text{Ln}=\text{Dy}, \text{Tb}, \text{Eu}, \text{Sm}, \text{Ho}$ ) clusters  
with different anion templates: magnetic and luminescent  
properties**

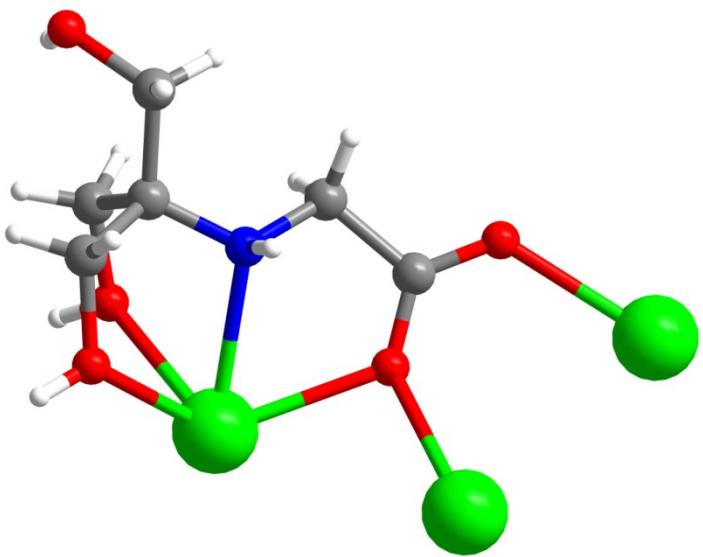
**Ying Zou,<sup>a</sup> Wei Lv,<sup>a</sup> Zhe Xue, Jie Pan,<sup>a</sup> Xiao-Yu Li,<sup>\*a</sup> and Guo-Ming Wang<sup>a</sup>**

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266071, P. R. China.*

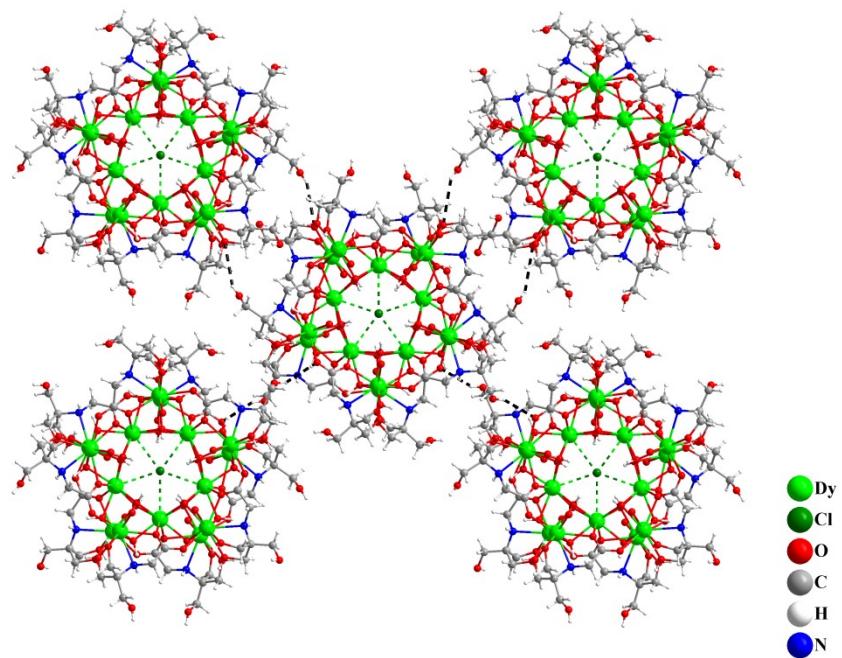
**Scheme S1: The syntheses route for clusters 1-5.**



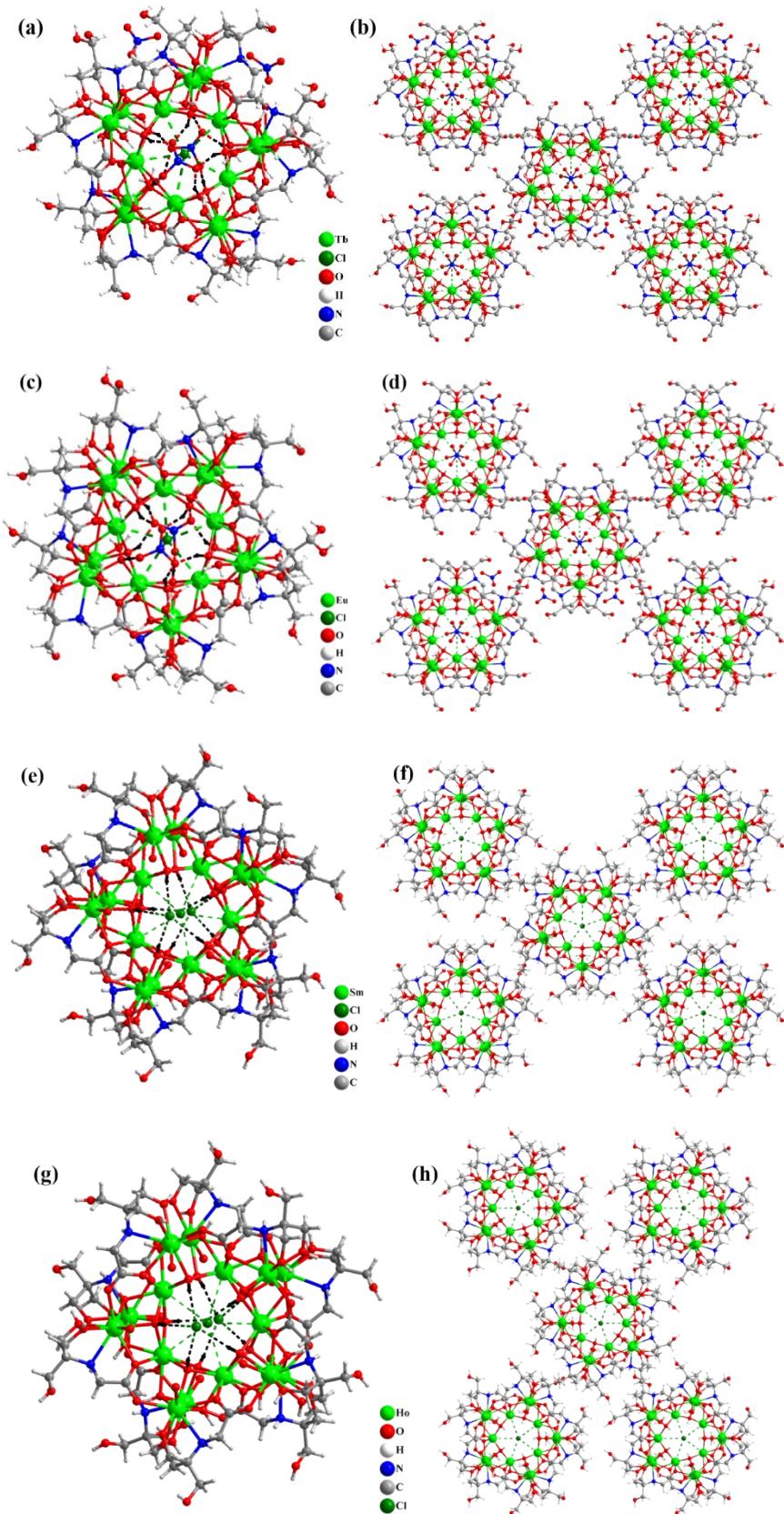
**Fig. S1: The coordination modes of H<sub>4</sub>thmmg<sup>-</sup> ligand in clusters 1-5.**



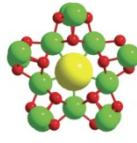
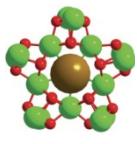
**Fig. S2:** The molecule packing of 1.

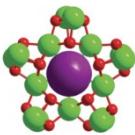


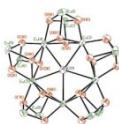
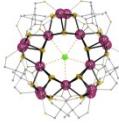
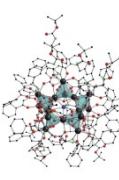
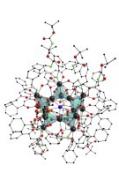
**Fig. S3: The molecular and packing structures of 2-5.**



**Table S1: The reported Ln<sub>15</sub> clusters**

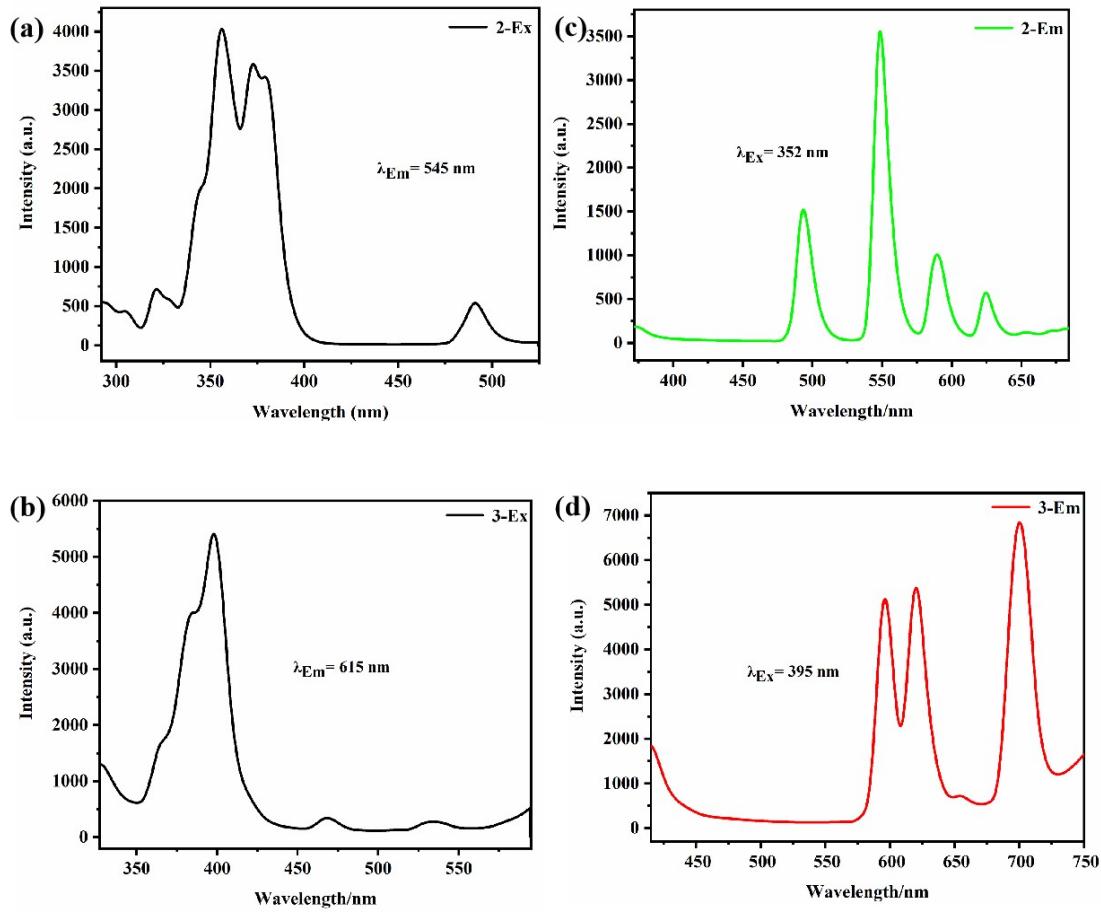
Structure	Chemical formula	Ligands	Anion template	cite
	[Nd <sub>15</sub> (μ <sub>5</sub> -Cl)(μ <sub>3</sub> -OH) <sub>20</sub> (His) <sub>10</sub> (H-His) <sub>5</sub> (H <sub>2</sub> O) <sub>9</sub> ] Cl <sub>4</sub> (ClO <sub>4</sub> ) <sub>10</sub> ·16H <sub>2</sub> O	L-histidine	Cl <sup>-</sup> ClO <sub>4</sub> <sup>-</sup>	<i>Inorg. Chem.</i> <i>Front. 2021</i> , 8, 26–34
	[Gd <sub>15</sub> (μ <sub>5</sub> -Cl)(μ <sub>3</sub> -OH) <sub>20</sub> (His) <sub>10</sub> (H-His) <sub>4</sub> (H <sub>2</sub> O) <sub>8</sub> ]Cl <sub>6</sub> (ClO <sub>4</sub> ) <sub>8</sub> ·22H <sub>2</sub> O			
	[Er <sub>15</sub> (μ <sub>5</sub> -Cl)(μ <sub>3</sub> -OH) <sub>20</sub> (His) <sub>10</sub> (H-His) <sub>4</sub> (H <sub>2</sub> O) <sub>6</sub> ]Cl <sub>4</sub> (ClO <sub>4</sub> ) <sub>10</sub> ·20H <sub>2</sub> O			
	[Nd <sub>15</sub> (μ <sub>5</sub> -Br)(μ <sub>3</sub> -OH) <sub>20</sub> (His) <sub>10</sub> (H-His) <sub>5</sub> (H <sub>2</sub> O) <sub>12</sub> ] Br <sub>3</sub> (ClO <sub>4</sub> ) <sub>11</sub> ·9H <sub>2</sub> O	L-histidine	Br <sup>-</sup> ClO <sub>4</sub> <sup>-</sup>	<i>Inorg. Chem.</i> <i>Front. 2021</i> , 8, 26–34
	[Gd <sub>15</sub> (μ <sub>5</sub> -Br)(μ <sub>3</sub> -OH) <sub>20</sub> (His) <sub>10</sub> (H-His) <sub>5</sub> (H <sub>2</sub> O) <sub>6</sub> ]Br <sub>4</sub> (ClO <sub>4</sub> ) <sub>10</sub> ·27H <sub>2</sub> O			
	[Er <sub>15</sub> (μ <sub>5</sub> -Br)(μ <sub>3</sub> -OH) <sub>20</sub> (His) <sub>10</sub> (H-His) <sub>4</sub> (H <sub>2</sub> O) <sub>6</sub> ]Br <sub>4</sub> (ClO <sub>4</sub> ) <sub>10</sub> ·24H <sub>2</sub> O			

	$\text{H}_2\text{O}$			
	$[\text{Nd}_{15}(\mu_5\text{-I})_{0.5}(\mu_5\text{-OH})_{0.5}(\mu_3\text{-OH})_{20}(\text{His})_{11}(\text{H-His})_4(\text{H}_2\text{O})_9]$  $\text{I}(\text{ClO}_4)_{12} \cdot 12\text{H}_2\text{O}$		$\text{I}^-$	
	$[\text{Nd}_{15}(\mu_3\text{-OH})_{20}(\mu_5\text{-Cl})(\mu_3\text{-Tyr})_{10}(\text{OH})_2(\mu_2\text{-H}_2\text{O})_5(\text{H}_2\text{O})_{18}] (\text{ClO}_4)_{12} \cdot 9\text{H}_2\text{O}$	L-Tyrosine	$\text{ClO}_4^-$	
	$[\text{Nd}_{15}(\mu_3\text{-OH})_{20}(\mu_5\text{-Cl})(\mu_3\text{-Tyr})_{10}(\text{OH})_3(\mu_2\text{-H}_2\text{O})(\text{H}_2\text{O})_{23}] \text{Cl}_3(\text{ClO}_4)_8 \cdot 2\text{H}_2\text{O}$		$\text{Cl}^-$	<i>Inorg. Chem.</i>
	$[\text{Gd}_{15}(\mu_3\text{-OH})_{20}(\mu_5\text{-Cl})(\mu_3\text{-Tyr})_{10}(\text{OH})(\mu_2\text{-H}_2\text{O})_5(\text{H}_2\text{O})_{19}] (\text{ClO}_4)_{13} \cdot 12\text{H}_2\text{O}$		$\text{ClO}_4^-$	2002, 41, 278–286
	$[\text{Pr}_{15}(\mu_3\text{-OH})_{20}(\mu_5\text{-Br})(\mu_3\text{-Tyr})_{10}(\mu_2\text{-TyrH})_2(\mu_2\text{-H}_2\text{O})_3(\text{H}_2\text{O})_{20}] (\text{ClO}_4)_{14} \cdot 8\text{H}_2\text{O}$		$\text{Br}^-$	
	$[\text{Eu}_{15}(\mu_3\text{-OH})_{20}(\mu_5\text{-Br})(\mu_3\text{-Tyr})_{10}(\mu_2\text{-H}_2\text{O})_5(\text{H}_2\text{O})_{19}] (\text{ClO}_4)_{13} \cdot 12\text{H}_2\text{O}$		$\text{ClO}_4^-$	

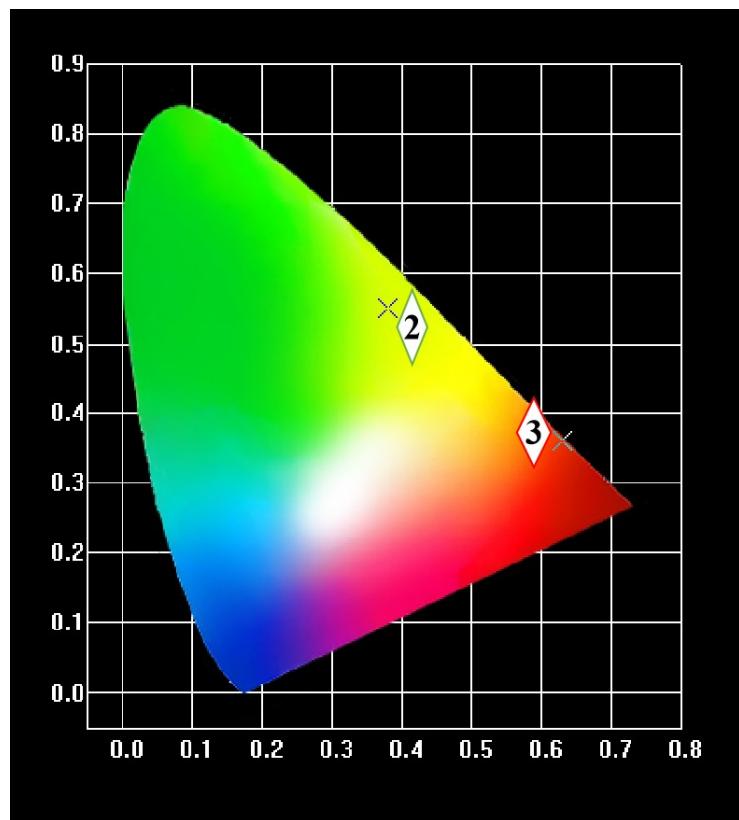
	$\text{H}_2\text{O})_5(\text{H}_2\text{O})_{20}](\text{ClO}_4)_{14}\cdot 2\text{H}_2\text{O}$			
	$[\text{Eu}_{15}(\text{Cl})(\mu_3\text{-Tyr})_{10}(\mu_3\text{-OH})_{20}(\mu_2\text{-H}_2\text{O})_5(\text{OH})_{12}(\text{H}_2\text{O})_8][\text{ClO}_4]_{2\cdot 56\text{H}_2\text{O}}$	L-Tyrosine	$\text{Cl}^-$ $\text{ClO}_4^-$	<i>Angew. Chem. Int. Ed.</i> 1999, 38, 1813-1815
	$[\text{Gd}_{15}(\mu_5\text{-Cl})(\text{OH})_{20}(\text{dmp})_{10}(\text{H}_2\text{O})_{10}](\text{ClO}_4)_8\text{Cl}_6$	2,2-dimethylolethylene propionic acid	$\text{Cl}^-$	<i>J. Am. Chem. Soc.</i> 2017, 139, 16405-16411
	$[\text{Er}_{15}(\mu_5\text{-Cl})(\mu_3\text{-OH})_{20}(\text{DMPA})_{12}(\text{H}_2\text{O})_6]\cdot (\text{ClO}_4)_{13}(\text{H}_2\text{O})_{24}$	2,2-dimethylolethylene propionic acid	$\text{Cl}^-$	<i>Inorg. Chem.</i> 2017, 56, 12821-12829
	$[\{\text{Y}_{15}(\text{OH})_{20}(\text{PepCO}_2)_{10}(\text{DBM})_{10}\text{Cl}\}\text{Cl}_4]$	(PepCO <sub>2</sub> =2-[{3-((tert-butoxycarbonyl)amino)methyl}benzyl]acetate, DBM=dibenzoylmethanide)	$\text{Cl}^-$	<i>Chem. Eur. J.</i> 2015, 21, 2813-2820
	$[\{\text{Dy}_{15}(\text{OH})_{20}(\text{PepCO}_2)_{10}(\text{DBM})_{10}\text{Cl}\}\text{Cl}_4]$			
	$[\text{Eu}_{15}(\mu_3\text{-OH})_{20}(\text{PepCO}_2)_{10}(\text{DBM})_{10}\text{Cl}]\text{Cl}_4$	(PepCO <sub>2</sub> =2-[{3-((tert-butoxycarbonyl)amino)methyl}benzyl]acetate, DBM=dibenzoylmethanide)	$\text{Cl}^-$	<i>J. Am. Chem. Soc.</i> 2013, 135, 7454-7457
	$[\text{Tb}_{15}(\mu_3\text{-OH})_{20}(\text{PepCO}_2)_{10}(\text{DBM})_{10}\text{Cl}]\text{Cl}_4$			

	Cl]Cl <sub>4</sub>			
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**Fig. S4: The emission and excitation spectra of the powder samples of 2 and 3 under room temperature.**



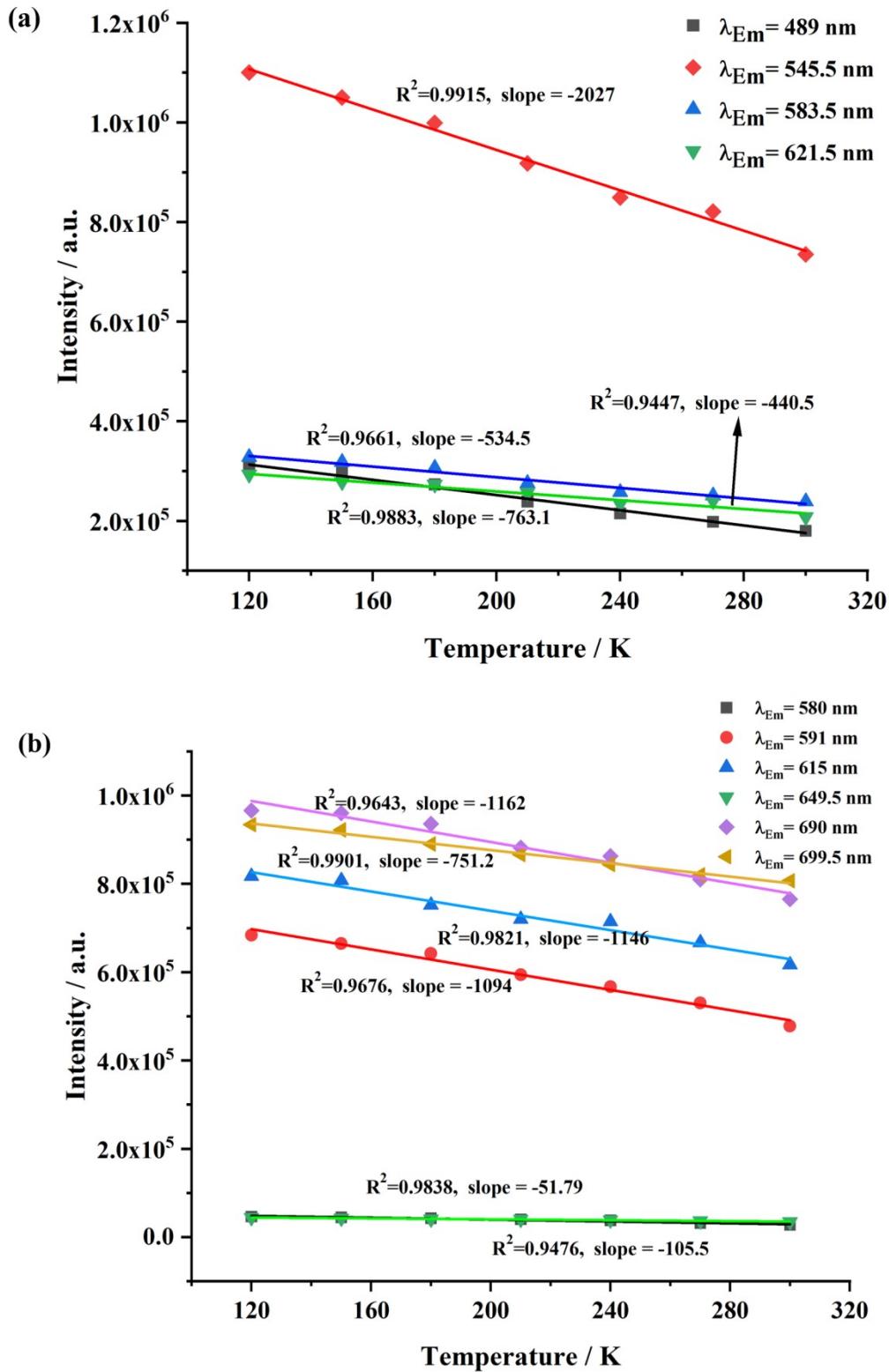
**Fig. S5: CIE chromatic coordinates of 2 and 3.**



**Table S2: The corresponding chromaticity coordinates of 2 and 3.**

	2		3	
	x	y	x	y
300K	0.3816	0.5496	0.6363	0.3601
270K	0.3806	0.5516	0.635	0.3612
240K	0.3793	0.5517	0.6345	0.3616
210K	0.3792	0.5534	0.6339	0.3624
180K	0.3793	0.5539	0.6335	0.3627
150K	0.3786	0.5542	0.6331	0.3632
120K	0.378	0.5551	0.6329	0.3634
90K	0.3767	0.5561	0.6328	0.3634

**Fig. S6: The linear fitting plots of maximum emission intensity vs. temperature of 2(a) and 3(b) in the range of 120 - 300 K.**



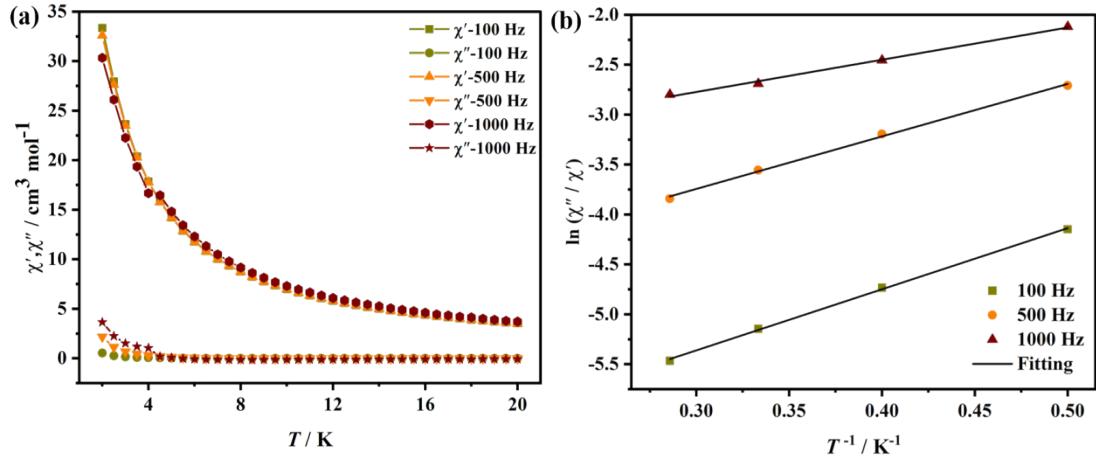
**Table S3: The comparison of quantum yields and luminescent lifetimes with other Tb/Eu clusters.**

Tb cluster	quantum yield	luminescent lifetime	cite
Tb <sub>2</sub>	47.1%	1072 μs	<i>Adv. Optical Mater.</i> 2022, 10, 2102267
Tb <sub>4</sub>	53%	1330 μs	<i>ACS Appl. Mater. Interfaces.</i> 2022, 14, 37894–37903
Tb <sub>5</sub>	-	1440 μs	<i>Polyhedron.</i> 2016, 106, 44–50
Tb <sub>6</sub>	17%	-	<i>Cryst. Growth Des.</i> 2012, 12, 970–974
Tb <sub>6</sub>	20.3%	18.63 μs	<i>Cryst. Growth Des.</i> 2018, 18, 1020–1029
Tb <sub>7</sub>	-	1441.8 μs	<i>Eur. J. Inorg. Chem.</i> 2017, 2700–2706
Tb <sub>9</sub>	8.1%	108.21 μs	<i>Cryst. Growth Des.</i> 2018, 18, 1020–1029
Tb <sub>12</sub>	0.39%	1.26 ns	<i>Inorg. Chem.</i> 2022, 61, 9385–9391
Tb <sub>14</sub>	-	797 μs	<i>Chem. Commun.</i> 2002, 368–369
Tb <sub>15</sub>	<3%	-	<i>J. Am. Chem. Soc.</i> 2013, 135, 7454–7457
Tb <sub>17</sub>	8.76%	1290 μs	<i>Inorg. Chem.</i> 2016, 55, 2037–2047
Tb <sub>20</sub>	-	605 μs	<i>Chem. Eur. J.</i> 2013, 19, 12254–12258
Tb <sub>48</sub>	3.11%	875 μs	<i>Cryst. Growth Des.</i> 2020, 20, 5294–5301
Tb <sub>15</sub>	58.05%	934 μs	This work

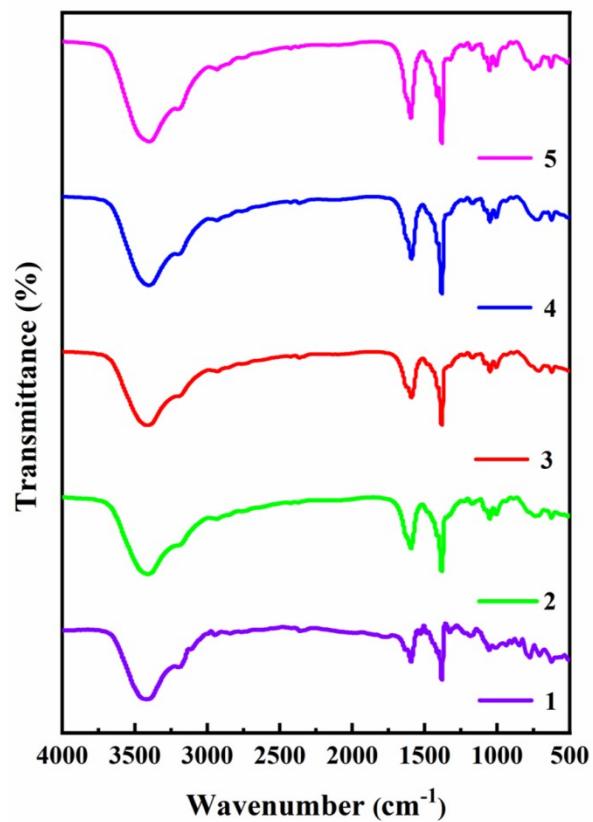
Eu cluster	quantum yield	luminescent lifetime	cite
Eu <sub>2</sub>	61.3%	424 μs	<i>Adv. Optical Mater.</i> 2022, 10, 2102267
Eu <sub>4</sub>	0.86%	25.07 ns	<i>ACS Appl. Mater. Interfaces.</i> 2022, 14, 37894–37903
Eu <sub>4</sub>	9.3%( <chem>CH3CN</chem> ), 4.0%( <chem>CH3OH</chem> ), 6.5%( <chem>CH3OD</chem> )	-	<i>Inorg. Chem.</i> 2007, 46, 7050–7054
Eu <sub>8</sub>	12.6%( <chem>CH3CN</chem> ), 7.1%( <chem>CH3OH</chem> ), 13.5%( <chem>CH3OD</chem> )	-	
Eu <sub>5</sub>	25%	660 μs	<i>Polyhedron.</i> 2016, 106, 44–50
Eu <sub>6</sub>	<10 <sup>-3</sup>	-	<i>Cryst. Growth Des.</i> 2012, 12, 970–974
Eu <sub>6</sub>	13.4%	35.76 μs	<i>Cryst. Growth Des.</i> 2018, 18, 1020–1029
Eu <sub>7</sub>	-	580.4 μs	<i>Eur. J. Inorg. Chem.</i> 2017, 2700–2706
Eu <sub>9</sub>	-	5.6 μs	<i>Cryst. Growth Des.</i> 2018, 18, 1020–1029
Eu <sub>9</sub>	11.6-19.8%	300-510 μs	<i>Inorg. Chem.</i> 2013, 52, 13332–13340
Eu <sub>12</sub>	-	120 μs	<i>Dalton Trans.</i> 2019, 48, 1700–1708
Eu <sub>14</sub>	-	345 μs	<i>Chem. Commun.</i> 2002, 368-369
Eu <sub>15</sub>	16%	-	<i>J. Am. Chem. Soc.</i> 2013, 135,

			7454–7457
Eu <sub>16</sub>	12.8%	361 μs	<i>J. Am. Chem. Soc.</i> 2022, 144, 5653–5660
Eu <sub>33</sub>	10.04%	194.7 μs	<i>Inorg. Chem.</i> 2022, 61, 8861–8869
Eu <sub>48</sub>	8.40%	287 μs	<i>Cryst. Growth Des.</i> 2020, 20, 5294–5301
Eu <sub>15</sub>	17.34%	242 μs	This work

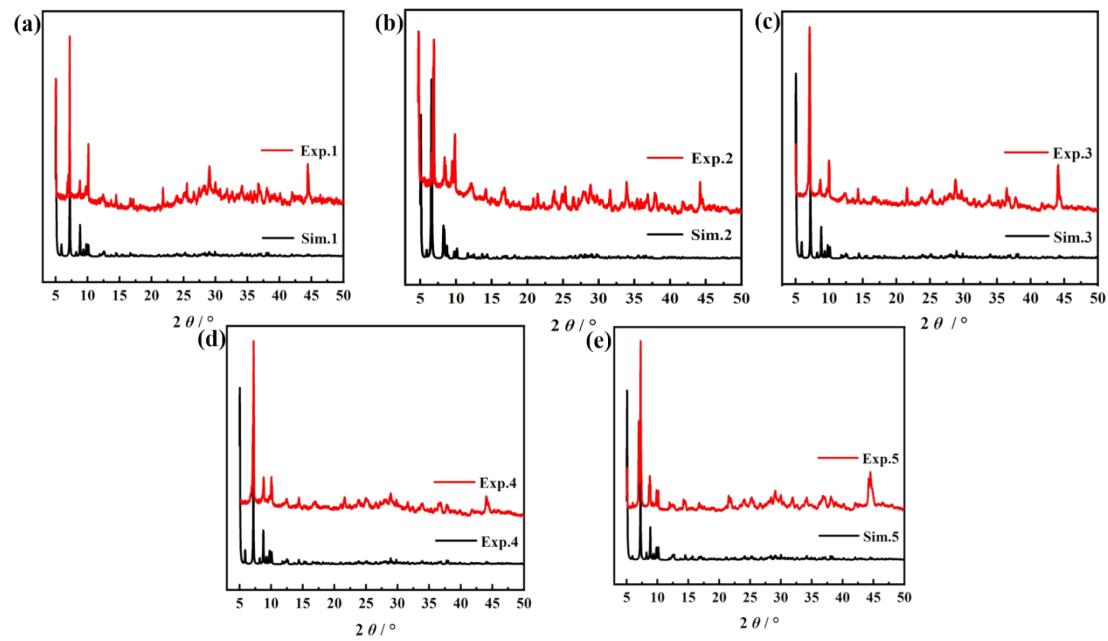
**Fig. S7: (a)The in- and out-of-phase ac susceptibilities for 1 under the zero dc field with different frequencies. (b) The  $\ln(\chi''/\chi')$ - $1/T$  plot of 1 and the gray lines represent the fitting results.**



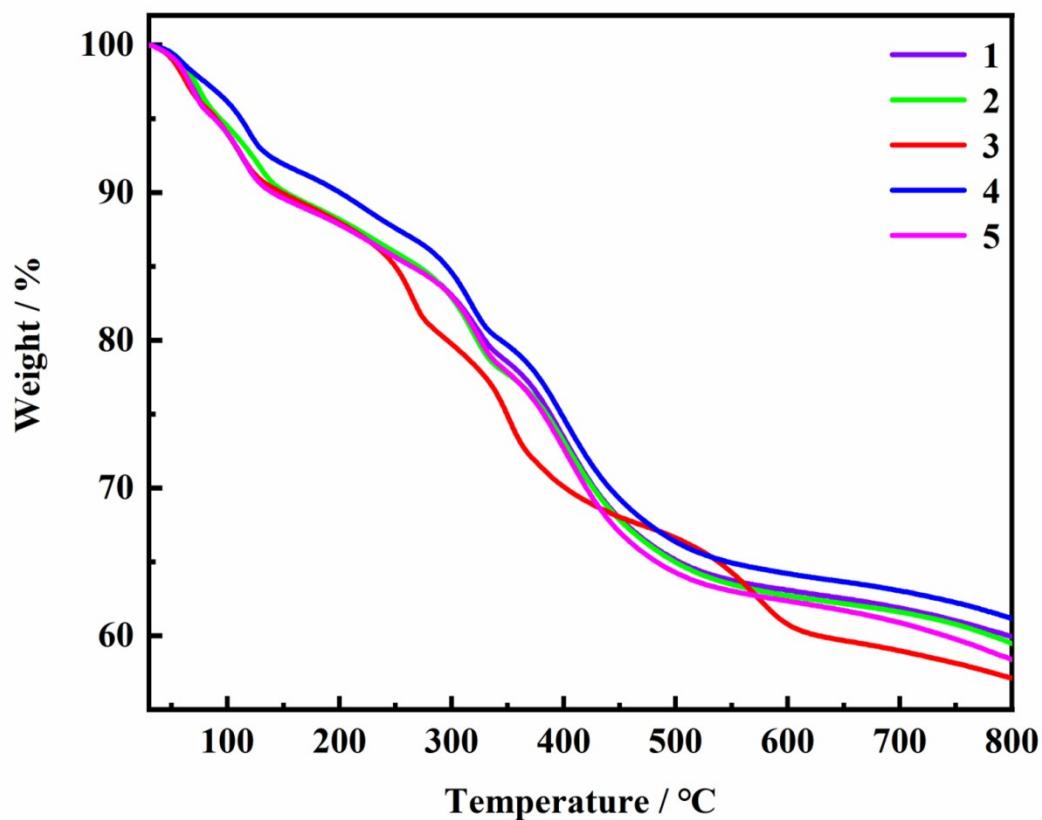
**Fig. S8:** The compared IR spectra of 1-5.



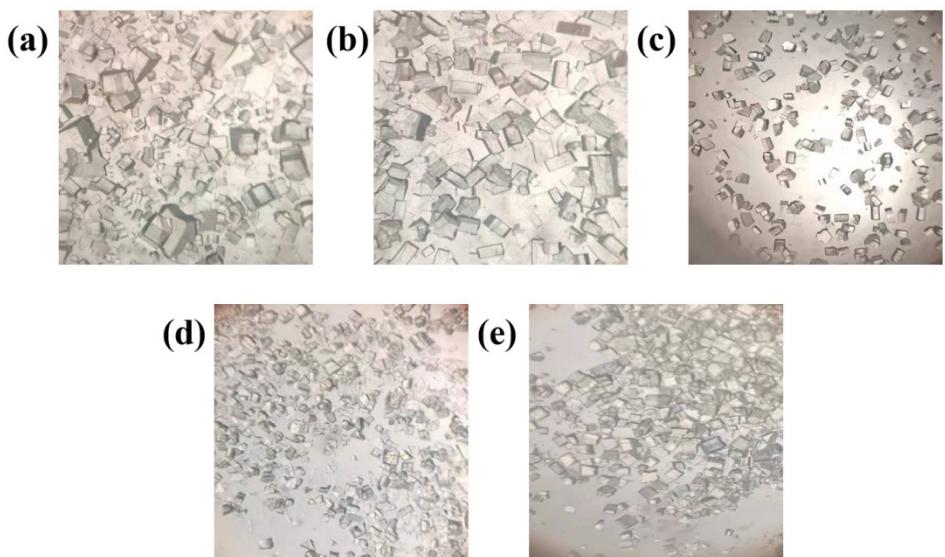
**Fig. S9: The PXRD of 1-5.**



**Fig. S10: The TGA of 1-5.**



**Fig. S11: Microscope photographs of crystals of 1(a), 2(b), 3(c), 4(d), and 5(e).**



**Table S4:** The hydrogen bond interactions of cluster **1**.

D-H	<i>d</i> (D-H)	<i>d</i> (H···A)	<D-H-A	<i>d</i> (D···A)	A
O8-H8	0.98	2.43	157	3.3500	C110 [ x, -y+1.5, -z+1 ]
O10-H10	0.98	2.40	157	3.3302	C110
O7-H7	0.98	2.45	155	3.3673	C110
O8-H8	0.98	2.42	158	3.3445	C110
O14-H14	0.98	2.43	157	3.3494	C110

**Table S5:** The hydrogen bond interactions of cluster **2**.

D-H	$d(\text{D-H})$	$d(\text{H}\cdots\text{A})$	$\angle\text{D-H-A}$	$d(\text{D}\cdots\text{A})$	A
O10-H10	1.00	1.86	159	2.8146	O39 [ -x+1, y, -z+0.5 ]
O7-H7	1.00	2.04	157	2.9828	O39
O2-H2	1.00	1.76	173	2.7570	O40 [ -x+1, y, -z+0.5 ]
O3-H3	1.00	2.04	155	2.9742	O41 [ -x+1, y, -z+0.5 ]
O2-H2	1.00	1.86	162	2.8293	O41

**Table S6: Crystal data for 1-5.**

Identification code	1	2	3	4	5
Empirical formula	C <sub>60</sub> H <sub>152</sub> Cl <sub>15</sub> Dy <sub>15</sub> N <sub>10</sub> O <sub>80</sub>	C <sub>60</sub> H <sub>160</sub> Cl <sub>11</sub> N <sub>14</sub> O <sub>92</sub> Tb <sub>15</sub>	C <sub>60</sub> H <sub>136</sub> Cl <sub>13</sub> Eu <sub>15</sub> N <sub>12</sub> O <sub>86</sub>	C <sub>60</sub> H <sub>144</sub> Cl <sub>15</sub> N <sub>10</sub> O <sub>80</sub> Sm <sub>15</sub>	C <sub>60</sub> H <sub>160</sub> Cl <sub>15</sub> Ho <sub>15</sub> N <sub>10</sub> O <sub>80</sub>
Formula weight	5227.71	5323.76	5071.15	4966.49	5307.67
Temperature/K	293(2)	100.00(10)	100.01(10)	293(2)	150.00(10)
Crystal system	<i>orthorhombic</i>	<i>monoclinic</i>	<i>orthorhombic</i>	<i>orthorhombic</i>	<i>orthorhombic</i>
Space group	<i>Pbcm</i>	<i>P2/c</i>	<i>Pmma</i>	<i>Pmma</i>	<i>Pbcm</i>
a/Å	21.5433(3)	13.4425(2)	29.9490(5)	30.0081(9)	21.4098(3)
b/Å	29.8188(3)	21.4389(4)	12.2649(2)	12.3183(3)	29.7523(4)
c/Å	24.4709(4)	29.9936(4)	21.5496(4)	21.6051(6)	24.2371(4)
α/°	90	90	90	90	90
β/°	90	91.4480(10)	90	90	90

$\gamma/^\circ$	90	90	90	90	90
Volume/ $\text{\AA}^3$	15720.0(4)	8641.2(2)	7915.6(2)	7986.3(4)	15438.8(4)
Z	4	2	2	2	4
$\rho_{\text{calc}} \text{g/cm}^3$	2.209	2.046	2.128	2.065	2.283
$\mu/\text{mm}^{-1}$	40.316	6.307	44.276	5.703	16.728
F(000)	9800	5032	4800	4696	9960
Radiation	Cu K $\alpha$ ( $\lambda = 1.54184$ )	Mo K $\alpha$ ( $\lambda = 0.71073$ )	Cu K $\alpha$ ( $\lambda = 1.54184$ )	Mo K $\alpha$ ( $\lambda = 0.71073$ )	Cu K $\alpha$ ( $\lambda = 1.54184$ )
2 $\Theta$ range for data collection/ $^\circ$	4.102 to 153.372	4.018 to 62.066	8.206 to 119.976	4.008 to 49.998	5.086 to 153.502
Index ranges	-27 $\leq h \leq 25$ , -37 $\leq k \leq 14$ , -30 $\leq l \leq 30$	-17 $\leq h \leq 18$ , -29 $\leq k \leq 25$ , -42 $\leq l \leq 34$	-33 $\leq h \leq 19$ , -13 $\leq k \leq 13$ , -24 $\leq l \leq 24$	-35 $\leq h \leq 33$ , -14 $\leq k \leq 13$ , -25 $\leq l \leq 20$	-25 $\leq h \leq 10$ , -37 $\leq k \leq 37$ , -30 $\leq l \leq 30$
Reflections collected	62120	101277	21655	33272	53272

Independent reflections	16305 [R <sub>int</sub> = 0.0844, R <sub>sigma</sub> = 0.0638]	22371 [R <sub>int</sub> = 0.0477, R <sub>sigma</sub> = 0.0395]	6296 [R <sub>int</sub> = 0.0589, R <sub>sigma</sub> = 0.0428]	7533 [R <sub>int</sub> = 0.0617, R <sub>sigma</sub> = 0.0411]	15720 [R <sub>int</sub> = 0.0906, R <sub>sigma</sub> = 0.0650]
Data/restraints/parameters	16305/376/846	22371/104/910	6296/525/650	7533/324/654	15720/128/860
Goodness-of-fit on F <sup>2</sup>	1.291	1.023	1.04	1.134	1.016
Final R indexes [I>=2σ (I)]	R <sub>1</sub> = 0.1042, wR <sub>2</sub> = 0.2998	R <sub>1</sub> = 0.0546, wR <sub>2</sub> = 0.1438	R <sub>1</sub> = 0.1036, wR <sub>2</sub> = 0.2709	R <sub>1</sub> = 0.0863, wR <sub>2</sub> = 0.2270	R <sub>1</sub> = 0.0955, wR <sub>2</sub> = 0.2620
Final R indexes [all data]	R <sub>1</sub> = 0.1218, wR <sub>2</sub> = 0.3187	R <sub>1</sub> = 0.0764, wR <sub>2</sub> = 0.1609	R <sub>1</sub> = 0.1089, wR <sub>2</sub> = 0.2756	R <sub>1</sub> = 0.1124, wR <sub>2</sub> = 0.2631	R <sub>1</sub> = 0.1120, wR <sub>2</sub> = 0.2855
Largest diff. peak/hole / e Å <sup>-3</sup>	4.63/-4.40	3.04/-2.05	3.82/-2.88	3.80/-2.54	4.80/-3.42



**Table S7: Selected bond distances (Å) and angles (°) for 1-5.**

1			
Dy1—Cl1	3.212 (4)	Dy5—O4	2.376 (8)
Dy1—O1	2.360 (9)	Dy5—N4	2.556 (10)
Dy1—O2	2.516 (9)	Dy5—O6	2.461 (9)
Dy1—O4	2.357 (8)	Dy5—O11	2.419 (8)
Dy1—O5	2.346 (9)	Dy5—O15	2.385 (8)
Dy1—O6	2.517 (9)	Dy5—O21 <sup>i</sup>	2.424 (9)
Dy1—O7	2.309 (8)	Dy5—O25	2.406 (12)
Dy1—O10	2.300 (8)	Dy5—O27	2.449 (14)
Dy1—O11	2.380 (9)	Dy6—O7	2.368 (8)
Dy2—O4	2.315 (8)	Dy6—O9	2.472 (9)
Dy2—O7	2.374 (8)	Dy6—O11	2.393 (9)
Dy2—O9	2.526 (10)	Dy6—O15	2.414 (9)
Dy2—O15	2.366 (9)	Dy6—O18	2.414 (10)
Dy3—O3	2.496 (9)	Dy6—O20	2.437 (10)
Dy3—O5	2.294 (8)	Dy6—O30	2.436 (13)
Dy3—O8 <sup>i</sup>	2.382 (9)	Dy7—O5	2.381 (8)
Dy3—O10	2.341 (8)	Dy7—N5	2.576 (13)
Dy3—O12	2.341 (8)	Dy7—O14	2.363 (8)
Dy3—O12 <sup>i</sup>	2.293 (7)	Dy7—O19	2.394 (10)
Dy3—O13	2.514 (9)	Dy7—O22	2.411 (10)
Dy3—O14	2.390 (9)	Dy7—O29	2.440 (12)
Dy4—N3	2.541 (15)	Dy8—Dy3 <sup>i</sup>	3.7760 (10)
Dy4—O10	2.372 (8)	Dy8—O8 <sup>i</sup>	2.416 (8)
Dy4—O13	2.436 (9)	Dy8—O8	2.355 (9)

Dy4—O14	2.432 (9)	Dy8—O12	2.374 (9)
Dy4—O17	2.405 (10)	Dy8—O16 <sup>i</sup>	2.426 (9)
Dy4—O23	2.411 (10)	Dy8—O24	2.392 (12)
Dy4—O26	2.434 (12)	Dy8—O28	2.430 (17)
O1—Dy1—Cl1	129.0 (3)	O6—Dy5—O2W	71.1 (4)
O1—Dy1—O2	67.9 (3)	O6—Dy5—N4	63.9 (3)
O1—Dy1—O6	76.7 (3)	O11—Dy5—O2W	134.9 (4)
O1—Dy1—O11	100.4 (3)	O11—Dy5—N4	77.9 (4)
O2—Dy1—Cl1	118.9 (2)	O11—Dy5—O6	68.6 (3)
O2—Dy1—O6	123.1 (3)	O11—Dy5—O21 <sup>i</sup>	140.1 (3)
O4—Dy1—Cl1	65.7 (3)	O11—Dy5—O27	138.6 (4)
O4—Dy1—O1	141.0 (3)	O15—Dy5—O2W	125.7 (4)
O4—Dy1—O2	143.3 (3)	O15—Dy5—N4	132.3 (4)
O4—Dy1—O6	65.9 (3)	O15—Dy5—O6	123.9 (3)
O4—Dy1—O11	76.3 (3)	O15—Dy5—O11	66.2 (3)
O5—Dy1—Cl1	64.8 (3)	O15—Dy5—O21 <sup>i</sup>	74.1 (3)
O5—Dy1—O1	75.7 (3)	O15—Dy5—O25	78.2 (4)
O5—Dy1—O2	66.9 (3)	O15—Dy5—O27	132.0 (4)
O5—Dy1—O4	130.4 (3)	O21 <sup>i</sup> —Dy5—O2W	73.5 (4)
O5—Dy1—O6	142.9 (3)	O21 <sup>i</sup> —Dy5—N4	130.3 (3)
O5—Dy1—O11	141.3 (3)	O21 <sup>i</sup> —Dy5—O6	144.2 (3)
O6—Dy1—Cl1	118.1 (2)	O21 <sup>i</sup> —Dy5—O27	68.8 (4)
O7—Dy1—Cl1	66.8 (3)	O25—Dy5—O2W	140.4 (5)
O7—Dy1—O1	145.4 (3)	O25—Dy5—N4	65.8 (4)
O7—Dy1—O2	77.6 (3)	O25—Dy5—O6	125.3 (4)
O7—Dy1—O4	71.5 (3)	O25—Dy5—O11	81.4 (4)
O7—Dy1—O5	89.3 (3)	O25—Dy5—O21 <sup>i</sup>	86.5 (4)

O7—Dy1—O6	126.9 (3)	O25—Dy5—O27	70.2 (5)
O7—Dy1—O11	72.1 (3)	O27—Dy5—O2W	70.8 (5)
O10—Dy1—Cl1	64.9 (3)	O27—Dy5—N4	63.3 (4)
O10—Dy1—O1	72.2 (3)	O27—Dy5—O6	103.9 (4)
O10—Dy1—O2	126.6 (3)	O1W—Dy6—N1	99.7 (4)
O10—Dy1—O4	89.3 (3)	O7—Dy6—O1W	72.5 (4)
O10—Dy1—O5	69.9 (3)	O7—Dy6—N1	128.8 (3)
O10—Dy1—O6	78.3 (3)	O7—Dy6—O9	67.3 (3)
O10—Dy1—O7	131.7 (3)	O7—Dy6—O11	70.9 (3)
O10—Dy1—O11	146.6 (3)	O7—Dy6—O15	75.3 (3)
O11—Dy1—Cl1	130.6 (3)	O7—Dy6—O18	146.6 (4)
O11—Dy1—O2	75.9 (3)	O7—Dy6—O20	95.8 (3)
O11—Dy1—O6	68.3 (3)	O7—Dy6—O30	142.2 (4)
O4 <sup>i</sup> —Dy2—O4	129.6 (4)	O9—Dy6—O1W	71.7 (4)
O4—Dy2—O7 <sup>i</sup>	88.0 (3)	O9—Dy6—N1	62.5 (3)
O4—Dy2—O7	71.0 (3)	O11—Dy6—O1W	126.7 (4)
O4—Dy2—O9	127.5 (3)	O11—Dy6—N1	133.5 (4)
O4 <sup>i</sup> —Dy2—O9	78.4 (3)	O11—Dy6—O9	124.3 (3)
O4 <sup>i</sup> —Dy2—O9 <sup>i</sup>	127.5 (3)	O11—Dy6—O15	66.2 (3)
O4—Dy2—O15 <sup>i</sup>	146.9 (3)	O11—Dy6—O18	78.8 (3)
O4 <sup>i</sup> —Dy2—O15	146.9 (3)	O11—Dy6—O20	73.5 (3)
O4—Dy2—O15	72.5 (3)	O11—Dy6—O30	130.8 (4)
O7 <sup>i</sup> —Dy2—O7	130.1 (4)	O15—Dy6—O1W	136.2 (4)
O7—Dy2—O9 <sup>i</sup>	143.6 (3)	O15—Dy6—N1	78.5 (4)
O7—Dy2—O9	66.3 (3)	O15—Dy6—O9	68.9 (3)
O9 <sup>i</sup> —Dy2—O9	123.0 (5)	O15—Dy6—O18	79.9 (4)
O15 <sup>i</sup> —Dy2—O7	140.6 (3)	O15—Dy6—O20	139.4 (3)

O15 <sup>i</sup> —Dy2—O7 <sup>i</sup>	76.1 (3)	O15—Dy6—O30	138.5 (4)
O15—Dy2—O9 <sup>i</sup>	76.2 (3)	O18—Dy6—O1W	139.6 (4)
O15—Dy2—O9	68.7 (3)	O18—Dy6—N1	65.6 (3)
O15 <sup>i</sup> —Dy2—O15	101.8 (4)	O18—Dy6—O9	123.3 (3)
O3—Dy3—Cl1	119.0 (2)	O18—Dy6—O20	88.5 (3)
O3—Dy3—O13	122.4 (3)	O18—Dy6—O30	69.8 (4)
O5—Dy3—Cl1	65.5 (2)	O20—Dy6—O1W	73.2 (4)
O5—Dy3—O3	79.3 (3)	O20—Dy6—N1	131.2 (4)
O5—Dy3—O8 <sup>i</sup>	147.5 (3)	O20—Dy6—O9	144.3 (3)
O5—Dy3—O10	70.1 (3)	O30—Dy6—O1W	70.0 (5)
O5—Dy3—O12	90.2 (3)	O30—Dy6—N1	63.6 (4)
O5—Dy3—O13	126.0 (3)	O30—Dy6—O9	104.6 (4)
O5—Dy3—O14	71.9 (3)	O30—Dy6—O20	68.9 (4)
O8 <sup>i</sup> —Dy3—Cl1	129.0 (3)	O1—Dy7—O2	67.7 (3)
O8 <sup>i</sup> —Dy3—O3	68.3 (3)	O1—Dy7—O5W	135.4 (4)
O8 <sup>i</sup> —Dy3—O13	76.3 (3)	O1—Dy7—N5	78.7 (3)
O8 <sup>i</sup> —Dy3—O14	101.6 (3)	O1—Dy7—O22	140.5 (3)
O10—Dy3—Cl1	64.9 (2)	O1—Dy7—O29	139.2 (3)
O10—Dy3—O3	143.8 (3)	O2—Dy7—N5	63.4 (3)
O10—Dy3—O8 <sup>i</sup>	140.7 (3)	O5W—Dy7—O2	71.9 (4)
O10—Dy3—O12	130.3 (3)	O5W—Dy7—N5	99.5 (4)
O10—Dy3—O13	66.4 (3)	O5—Dy7—O1	74.1 (3)
O10—Dy3—O14	76.1 (3)	O5—Dy7—O2	67.0 (3)
O12 <sup>i</sup> —Dy3—Cl1	65.8 (3)	O5—Dy7—O5W	73.5 (4)
O12—Dy3—Cl1	65.4 (2)	O5—Dy7—N5	129.3 (3)
O12 <sup>i</sup> —Dy3—O3	126.5 (3)	O5—Dy7—O19	147.1 (4)
O12—Dy3—O3	66.7 (3)	O5—Dy7—O22	96.1 (3)

O12 <sup>i</sup> —Dy3—O5	131.3 (3)	O5—Dy7—O29	144.0 (4)
O12 <sup>i</sup> —Dy3—O8 <sup>i</sup>	71.2 (3)	O14—Dy7—O1	66.3 (3)
O12—Dy3—O8 <sup>i</sup>	75.3 (3)	O14—Dy7—O2	123.9 (3)
O12 <sup>i</sup> —Dy3—O10	88.9 (3)	O14—Dy7—O5W	127.7 (4)
O12 <sup>i</sup> —Dy3—O12	70.4 (4)	O14—Dy7—O5	70.9 (3)
O12 <sup>i</sup> —Dy3—O13	78.2 (3)	O14—Dy7—N5	132.7 (4)
O12—Dy3—O13	142.9 (3)	O14—Dy7—O19	78.9 (3)
O12 <sup>i</sup> —Dy3—O14	146.1 (3)	O14—Dy7—O22	74.3 (3)
O12—Dy3—O14	141.5 (3)	O14—Dy7—O29	127.8 (4)
O13—Dy3—Cl1	118.6 (2)	O19—Dy7—O1	82.2 (4)
O14—Dy3—Cl1	129.5 (3)	O19—Dy7—O2	124.0 (3)
O14—Dy3—O3	76.4 (3)	O19—Dy7—O5W	138.0 (4)
O14—Dy3—O13	67.9 (3)	O19—Dy7—N5	65.2 (4)
O1—Dy4—O3W	125.6 (4)	O19—Dy7—O22	87.9 (4)
O1—Dy4—N3	131.6 (4)	O19—Dy7—O29	66.8 (4)
O1—Dy4—O13	123.3 (3)	O22—Dy7—O2	144.0 (3)
O1—Dy4—O14	65.4 (3)	O22—Dy7—O5W	72.8 (4)
O1—Dy4—O17	74.2 (3)	O22—Dy7—N5	130.5 (3)
O1—Dy4—O23	79.4 (4)	O22—Dy7—O29	66.6 (4)
O1—Dy4—O26	133.7 (4)	O29—Dy7—O2	108.0 (4)
O3W—Dy4—N3	102.7 (5)	O29—Dy7—O5W	71.3 (5)
O10—Dy4—O1	70.2 (3)	O29—Dy7—N5	64.8 (4)
O10—Dy4—O3W	72.0 (4)	O4W—Dy8—N2	99.5 (4)
O10—Dy4—N3	130.0 (4)	O4W—Dy8—O3	72.7 (3)
O10—Dy4—O13	67.2 (3)	O3—Dy8—N2	63.4 (3)
O10—Dy4—O14	74.7 (3)	O8—Dy8—O4W	126.8 (4)
O10—Dy4—O17	97.0 (3)	O8 <sup>i</sup> —Dy8—O4W	136.2 (4)

O10—Dy4—O23	148.0 (4)	O8 <sup>i</sup> —Dy8—N2	79.8 (4)
O10—Dy4—O26	140.9 (4)	O8—Dy8—N2	133.6 (4)
O13—Dy4—O3W	72.7 (4)	O8 <sup>i</sup> —Dy8—O3	68.0 (3)
O13—Dy4—N3	64.0 (4)	O8—Dy8—O3	122.6 (3)
O14—Dy4—O3W	136.1 (4)	O8—Dy8—O8 <sup>i</sup>	65.2 (4)
O14—Dy4—N3	78.0 (4)	O8—Dy8—O12	70.3 (3)
O14—Dy4—O13	68.5 (3)	O8 <sup>i</sup> —Dy8—O16 <sup>i</sup>	138.3 (3)
O14—Dy4—O26	139.1 (3)	O8—Dy8—O16 <sup>i</sup>	73.5 (3)
O17—Dy4—O3W	73.2 (4)	O8—Dy8—O24	79.5 (4)
O17—Dy4—N3	130.0 (4)	O8 <sup>i</sup> —Dy8—O28	139.7 (4)
O17—Dy4—O13	145.5 (3)	O8—Dy8—O28	131.7 (4)
O17—Dy4—O14	139.2 (3)	O12—Dy8—O4W	73.1 (4)
O17—Dy4—O23	83.9 (4)	O12—Dy8—N2	129.1 (3)
O17—Dy4—O26	69.4 (4)	O12—Dy8—O3	66.5 (3)
O23—Dy4—O3W	137.3 (5)	O12—Dy8—O8 <sup>i</sup>	74.1 (3)
O23—Dy4—N3	65.6 (5)	O12—Dy8—O16 <sup>i</sup>	97.0 (3)
O23—Dy4—O13	126.1 (4)	O12—Dy8—O24	147.0 (4)
O23—Dy4—O14	83.8 (4)	O12—Dy8—O28	142.1 (5)
O23—Dy4—O26	69.3 (4)	O16 <sup>i</sup> —Dy8—O4W	74.2 (3)
O26—Dy4—O3W	69.0 (4)	O16 <sup>i</sup> —Dy8—N2	130.2 (4)
O26—Dy4—N3	63.1 (5)	O16 <sup>i</sup> —Dy8—O3	146.1 (3)
O26—Dy4—O13	102.8 (4)	O16 <sup>i</sup> —Dy8—O28	68.7 (4)
O2W—Dy5—N4	101.8 (4)	O24—Dy8—O4W	138.5 (5)
O4—Dy5—O2W	70.8 (4)	O24—Dy8—N2	65.5 (4)
O4—Dy5—N4	129.3 (3)	O24—Dy8—O3	123.7 (3)
O4—Dy5—O6	66.5 (3)	O24—Dy8—O8 <sup>i</sup>	81.4 (4)
O4—Dy5—O11	75.2 (3)	O24—Dy8—O16 <sup>i</sup>	86.7 (3)

O4—Dy5—O15	71.1 (3)	O24—Dy8—O28	69.5 (6)
O4—Dy5—O21 <sup>i</sup>	96.7 (3)	O28—Dy8—O4W	69.3 (6)
O4—Dy5—O25	146.9 (4)	O28—Dy8—N2	63.2 (4)
O4—Dy5—O27	141.4 (4)	O28—Dy8—O3	105.5 (4)

Symmetry code: (i)  $x, -y+3/2, -z+1$ .

## 2

Tb1—O1	2.377 (5)	Tb4—O31	2.445 (7)
Tb1—O2	2.372 (6)	Tb5—O5	2.380 (6)
Tb1—O3	2.323 (5)	Tb5—O6	2.412 (5)
Tb1—O27	2.515 (6)	Tb5—O7	2.321 (6)
C11—Tb3	3.1972 (11)	Tb5—O9	2.391 (6)
C11—Tb5	3.216 (3)	Tb5—O10 <sup>i</sup>	2.325 (5)
O1—Tb2	2.406 (6)	Tb5—O10	2.379 (5)
O1—Tb4	2.400 (6)	Tb5—O11	2.477 (6)
Tb2—O3	2.342 (5)	Tb5—O17	2.505 (6)
Tb2—O4	2.441 (7)	Tb6—O6	2.434 (7)
Tb2—O4W	2.476 (8)	Tb6—O8	2.400 (6)
Tb2—O22	2.481 (6)	Tb6—O17	2.473 (6)
Tb2—O23	2.395 (7)	Tb6—O18	2.443 (8)
Tb2—O24	2.445 (8)	Tb6—O19	2.444 (7)
Tb2—O26	2.437 (7)	Tb6—O21	2.416 (7)
Tb3—O3	2.374 (6)	Tb7—O9 <sup>i</sup>	2.395 (6)
Tb3—O4	2.400 (6)	Tb7—O9	2.410 (6)
Tb3—O5	2.323 (5)	Tb7—O10	2.351 (6)
Tb3—O7	2.387 (6)	Tb7—O11	2.502 (6)
Tb3—O8	2.388 (6)	Tb7—O13	2.475 (9)
Tb3—O22	2.533 (6)	Tb7—O14	2.466 (9)

Tb3—O32	2.489 (6)	Tb7—O16 <sup>i</sup>	2.450 (7)
Tb4—O4	2.366 (6)	Tb8—O8	2.407 (6)
Tb4—N5 <sup>i</sup>	2.562 (8)	Tb8—O12	2.448 (7)
Tb4—O27 <sup>i</sup>	2.501 (6)	Tb8—O32	2.488 (6)
Tb4—O28 <sup>i</sup>	2.470 (11)	Tb8—O33	2.445 (8)
Tb4—O29 <sup>i</sup>	2.466 (9)	Tb8—O34	2.472 (8)
O1—Tb1—O1 <sup>i</sup>	100.8 (3)	O7—Tb5—O10	90.6 (2)
O1 <sup>i</sup> —Tb1—O27	68.1 (2)	O7—Tb5—O10 <sup>i</sup>	134.6 (2)
O1 <sup>i</sup> —Tb1—O27 <sup>i</sup>	74.5 (2)	O7—Tb5—O11	77.6 (2)
O1—Tb1—O27	74.5 (2)	O7—Tb5—O17	126.0 (2)
O1—Tb1—O27 <sup>i</sup>	68.1 (2)	O9—Tb5—Cl1	129.33 (14)
O2 <sup>i</sup> —Tb1—O1	138.9 (2)	O9—Tb5—O6	101.4 (2)
O2—Tb1—O1	75.0 (2)	O9—Tb5—O11	67.6 (2)
O2 <sup>i</sup> —Tb1—O1 <sup>i</sup>	75.0 (2)	O9—Tb5—O17	76.2 (2)
O2—Tb1—O1 <sup>i</sup>	138.9 (2)	O10 <sup>i</sup> —Tb5—Cl1	67.03 (14)
O2 <sup>i</sup> —Tb1—O2	134.4 (3)	O10—Tb5—Cl1	66.54 (14)
O2 <sup>i</sup> —Tb1—O27	65.88 (19)	O10—Tb5—O5	132.35 (19)
O2 <sup>i</sup> —Tb1—O27 <sup>i</sup>	142.9 (2)	O10 <sup>i</sup> —Tb5—O5	89.69 (19)
O3 <sup>i</sup> —Tb1—O1	146.8 (2)	O10—Tb5—O6	140.9 (2)
O3—Tb1—O1	71.48 (19)	O10 <sup>i</sup> —Tb5—O6	144.9 (2)
O3—Tb1—O2	71.9 (2)	O10 <sup>i</sup> —Tb5—O9	70.9 (2)
O3—Tb1—O2 <sup>i</sup>	89.76 (19)	O10—Tb5—O9	74.5 (2)
O3 <sup>i</sup> —Tb1—O2 <sup>i</sup>	71.9 (2)	O10 <sup>i</sup> —Tb5—O10	71.8 (2)
O3 <sup>i</sup> —Tb1—O2	89.76 (19)	O10—Tb5—O11	66.3 (2)
O3 <sup>i</sup> —Tb1—O3	132.0 (3)	O10 <sup>i</sup> —Tb5—O11	126.8 (2)
O3—Tb1—O27 <sup>i</sup>	127.14 (19)	O10—Tb5—O17	143.1 (2)
O3 <sup>i</sup> —Tb1—O27 <sup>i</sup>	78.7 (2)	O10 <sup>i</sup> —Tb5—O17	77.7 (2)

O27 <sup>i</sup> —Tb1—O27	119.8 (3)	O11—Tb5—Cl1	119.67 (15)
O1—Tb2—O4	65.0 (2)	O11—Tb5—O17	121.0 (2)
O1—Tb2—O4W	127.8 (2)	O17—Tb5—Cl1	119.31 (15)
O1—Tb2—O22	122.7 (2)	O3W—Tb6—N2	99.7 (3)
O1—Tb2—O24	134.2 (3)	O3W—Tb6—O17	72.8 (2)
O1—Tb2—O26	73.6 (2)	O5—Tb6—N2	129.8 (2)
O3—Tb2—O1	70.66 (19)	O5—Tb6—O3W	73.8 (2)
O3—Tb2—O4	74.4 (2)	O5—Tb6—O6	75.1 (2)
O3—Tb2—N4	129.3 (2)	O5—Tb6—O8	70.09 (19)
O3—Tb2—O22	67.11 (18)	O5—Tb6—O17	67.37 (19)
O3—Tb2—O23	147.0 (2)	O5—Tb6—O18	139.8 (3)
O3—Tb2—O24	140.5 (3)	O5—Tb6—O19	148.7 (2)
O3—Tb2—O26	97.6 (2)	O5—Tb6—O21	97.7 (2)
O4—Tb2—O4W	136.2 (2)	O6—Tb6—N2	78.0 (3)
O4—Tb2—O22	67.6 (2)	O6—Tb6—O3W	136.4 (2)
O4—Tb2—O24	139.4 (2)	O6—Tb6—O17	67.4 (2)
O4W—Tb2—O22	73.0 (3)	O6—Tb6—O18	139.5 (3)
O22—Tb2—N4	63.4 (2)	O6—Tb6—O19	84.2 (3)
O23—Tb2—O1	77.7 (2)	O8—Tb6—N2	132.0 (3)
O23—Tb2—O4	84.2 (3)	O8—Tb6—O3W	128.1 (3)
O23—Tb2—O4W	136.6 (3)	O8—Tb6—O6	65.4 (2)
O23—Tb2—N4	67.2 (2)	O8—Tb6—O17	122.3 (2)
O23—Tb2—O22	126.9 (2)	O8—Tb6—O18	134.4 (3)
O23—Tb2—O24	70.4 (3)	O8—Tb6—O19	80.1 (2)
O23—Tb2—O26	81.8 (3)	O8—Tb6—O21	73.2 (2)
O24—Tb2—O4W	67.3 (3)	O17—Tb6—N2	63.3 (2)
O24—Tb2—N4	63.8 (3)	O18—Tb6—N2	63.5 (3)

O24—Tb2—O22	102.8 (3)	O18—Tb6—O3W	66.3 (3)
O26—Tb2—O4	138.2 (2)	O18—Tb6—O17	103.1 (3)
O26—Tb2—O4W	75.1 (3)	O18—Tb6—O19	69.6 (3)
O26—Tb2—N4	130.7 (2)	O19—Tb6—N2	65.9 (2)
O26—Tb2—O22	147.5 (2)	O19—Tb6—O3W	135.2 (3)
O26—Tb2—O24	70.1 (2)	O19—Tb6—O17	125.4 (2)
O2—Tb3—O3	71.9 (2)	O21—Tb6—N2	129.8 (2)
O2—Tb3—O4	70.2 (2)	O21—Tb6—O3W	76.3 (3)
O2—Tb3—O5	135.39 (19)	O21—Tb6—O6	138.0 (2)
O2—Tb3—O7	92.5 (2)	O21—Tb6—O17	148.4 (2)
O2—Tb3—O8	145.9 (2)	O21—Tb6—O18	69.7 (3)
O2—Tb3—O22	126.0 (2)	O21—Tb6—O19	82.2 (3)
O2—Tb3—O32	78.4 (2)	O1W—Tb7—N1	96.9 (3)
O3—Tb3—Cl1	66.56 (13)	O1W—Tb7—O11	71.7 (3)
O3—Tb3—O4	74.6 (2)	O1W—Tb7—O13	136.0 (4)
O3—Tb3—O7	133.89 (18)	O1W—Tb7—O14	69.1 (4)
O3—Tb3—O8	139.1 (2)	O1W—Tb7—O16 <sup>i</sup>	75.2 (3)
O3—Tb3—O22	65.80 (19)	O9—Tb7—O1W	135.5 (3)
O3—Tb3—O32	143.89 (19)	O9 <sup>i</sup> —Tb7—O1W	129.9 (3)
O4—Tb3—O22	67.4 (2)	O9 <sup>i</sup> —Tb7—N1	133.0 (3)
O4—Tb3—O32	76.4 (2)	O9—Tb7—N1	78.7 (3)
O5—Tb3—Cl1	66.66 (14)	O9 <sup>i</sup> —Tb7—O9	65.3 (2)
O5—Tb3—O3	89.5 (2)	O9 <sup>i</sup> —Tb7—O11	121.7 (2)
O5—Tb3—O4	144.2 (2)	O9—Tb7—O11	66.9 (2)
O5—Tb3—O7	71.4 (2)	O9 <sup>i</sup> —Tb7—O13	80.8 (3)
O5—Tb3—O8	70.65 (19)	O9—Tb7—O13	82.3 (3)
O5—Tb3—O22	76.86 (19)	O9—Tb7—O14	140.1 (3)

O5—Tb3—O32	126.4 (2)	O9 <sup>i</sup> —Tb7—O14	129.2 (4)
O7—Tb3—Cl1	67.34 (14)	O9—Tb7—O16 <sup>i</sup>	139.0 (2)
O7—Tb3—O4	141.4 (2)	O9 <sup>i</sup> —Tb7—O16 <sup>i</sup>	73.8 (2)
O7—Tb3—O8	74.2 (2)	O10—Tb7—O1W	74.4 (3)
O7—Tb3—O22	141.30 (19)	O10—Tb7—N1	128.7 (2)
O7—Tb3—O32	66.3 (2)	O10—Tb7—O9 <sup>i</sup>	70.4 (2)
O8—Tb3—O4	100.63 (19)	O10—Tb7—O9	74.7 (2)
O8—Tb3—O22	74.8 (2)	O10—Tb7—O11	66.29 (19)
O8—Tb3—O32	67.4 (2)	O10—Tb7—O13	148.6 (3)
O32—Tb3—O22	120.5 (2)	O10—Tb7—O14	142.4 (4)
O32—Tb3—Cl1	120.65 (16)	O10—Tb7—O16 <sup>i</sup>	95.4 (2)
O1—Tb4—O2W	137.3 (3)	O11—Tb7—N1	63.1 (2)
O1—Tb4—N5 <sup>i</sup>	79.3 (3)	O13—Tb7—N1	64.8 (3)
O1—Tb4—O27 <sup>i</sup>	68.0 (2)	O13—Tb7—O11	123.2 (3)
O1—Tb4—O28 <sup>i</sup>	77.4 (3)	O14—Tb7—N1	65.8 (3)
O1—Tb4—O29 <sup>i</sup>	136.8 (3)	O14—Tb7—O11	108.9 (4)
O1—Tb4—O31	139.7 (2)	O14—Tb7—O13	67.0 (4)
O2—Tb4—O1	74.7 (2)	O16 <sup>i</sup> —Tb7—N1	131.9 (3)
O2—Tb4—O2W	77.7 (3)	O16 <sup>i</sup> —Tb7—O11	145.4 (2)
O2—Tb4—O4	70.1 (2)	O16 <sup>i</sup> —Tb7—O13	88.1 (3)
O2—Tb4—N5 <sup>i</sup>	128.1 (2)	O16 <sup>i</sup> —Tb7—O14	67.1 (3)
O2—Tb4—O27 <sup>i</sup>	66.27 (19)	O5W—Tb8—N3	95.4 (3)
O2—Tb4—O28 <sup>i</sup>	145.4 (3)	O5W—Tb8—O12	74.8 (3)
O2—Tb4—O29 <sup>i</sup>	147.6 (4)	O5W—Tb8—O32	71.6 (3)
O2—Tb4—O31	93.5 (2)	O5W—Tb8—O33	70.7 (4)
O2W—Tb4—N5 <sup>i</sup>	93.1 (3)	O5W—Tb8—O34	137.4 (3)
O2W—Tb4—O27 <sup>i</sup>	71.3 (3)	O6—Tb8—N3	134.2 (3)

O2W—Tb4—O28 <sup>i</sup>	136.7 (4)	O6—Tb8—O5W	130.3 (3)
O2W—Tb4—O29 <sup>i</sup>	72.1 (4)	O6—Tb8—O8	66.0 (2)
O2W—Tb4—O31	73.4 (3)	O6—Tb8—O12	72.8 (2)
O4—Tb4—O1	66.2 (2)	O6—Tb8—O32	122.8 (2)
O4—Tb4—O2W	131.5 (3)	O6—Tb8—O33	125.2 (3)
O4—Tb4—N5 <sup>i</sup>	135.3 (3)	O6—Tb8—O34	80.2 (2)
O4—Tb4—O27 <sup>i</sup>	122.8 (2)	O7—Tb8—N3	129.5 (2)
O4—Tb4—O28 <sup>i</sup>	80.2 (3)	O7—Tb8—O5W	75.2 (3)
O4—Tb4—O29 <sup>i</sup>	123.5 (3)	O7—Tb8—O6	70.58 (19)
O4—Tb4—O31	73.5 (2)	O7—Tb8—O8	74.7 (2)
O27 <sup>i</sup> —Tb4—N5 <sup>i</sup>	62.5 (2)	O7—Tb8—O12	94.0 (2)
O28 <sup>i</sup> —Tb4—N5 <sup>i</sup>	64.6 (3)	O7—Tb8—O32	66.95 (19)
O28 <sup>i</sup> —Tb4—O27 <sup>i</sup>	120.4 (3)	O7—Tb8—O33	143.9 (3)
O29 <sup>i</sup> —Tb4—N5 <sup>i</sup>	66.0 (3)	O7—Tb8—O34	147.0 (3)
O29 <sup>i</sup> —Tb4—O27 <sup>i</sup>	113.2 (3)	O8—Tb8—N3	79.9 (3)
O29 <sup>i</sup> —Tb4—O28 <sup>i</sup>	65.1 (5)	O8—Tb8—O5W	135.8 (2)
O31—Tb4—N5 <sup>i</sup>	133.0 (2)	O8—Tb8—O12	138.8 (2)
O31—Tb4—O27 <sup>i</sup>	142.2 (2)	O8—Tb8—O32	67.2 (2)
O31—Tb4—O28 <sup>i</sup>	94.7 (3)	O8—Tb8—O33	140.0 (3)
O31—Tb4—O29 <sup>i</sup>	67.0 (3)	O8—Tb8—O34	79.6 (3)
O5—Tb5—O6	74.9 (2)	O12—Tb8—N3	131.9 (3)
O5—Tb5—O9	140.8 (2)	O12—Tb8—O32	144.5 (2)
O5—Tb5—O11	143.1 (2)	O12—Tb8—O34	91.8 (3)
O5—Tb5—O17	66.3 (2)	O32—Tb8—N3	63.1 (2)
O6—Tb5—O11	76.1 (2)	O33—Tb8—N3	66.3 (3)
O6—Tb5—O17	67.2 (2)	O33—Tb8—O12	66.1 (3)
O7—Tb5—Cl1	67.59 (14)	O33—Tb8—O32	111.6 (3)

O7—Tb5—O5	71.6 (2)	O33—Tb8—O34	67.0 (4)
O7—Tb5—O6	70.47 (19)	O34—Tb8—N3	63.7 (3)
O7—Tb5—O9	145.1 (2)	O34—Tb8—O32	120.8 (3)

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

### 3

Eu1—O19	2.360 (10)	Eu3—O18	2.385 (16)
Eu1—O20	2.430 (10)	Eu3—O11	2.498 (17)
Eu1—O18	2.421 (9)	Eu3—O16	2.422 (14)
Eu1—O2W	2.524 (15)	Eu4—Cl1	3.208 (3)
Eu1—O9	2.425 (18)	Eu4—O19	2.384 (11)
Eu1—O10	3.050 (19)	Eu4—O22	2.387 (10)
Eu1—O11	3.017 (18)	Eu4—O20	2.402 (18)
Eu1—O8	2.488 (18)	Eu4—O21	2.420 (15)
Eu1—N2A	2.77 (4)	Eu4—O10 <sup>iii</sup>	2.534 (14)
Eu1—N2	2.72 (4)	Eu5—O22	2.370 (10)
Eu2—O17	2.347 (15)	Eu5—O23 <sup>ii</sup>	2.421 (10)
Eu2—O1W	2.49 (2)	Eu5—O21	2.434 (9)
Eu2—O15	2.45 (3)	Eu5—O3W	2.507 (14)
Eu2—O11 <sup>i</sup>	3.044 (18)	Eu5—O10	3.021 (19)
Eu2—O11	3.044 (18)	Eu5—O2	2.442 (16)
Eu2—O16	2.406 (9)	Eu5—O5	3.030 (3)
Eu2—O16 <sup>ii</sup>	2.406 (9)	Eu5—O3	2.479 (16)
Eu2—O14	2.50 (2)	Eu5—N1A	2.74 (3)
Eu2—N3 <sup>i</sup>	2.74 (5)	Eu5—N1	2.72 (4)
Eu2—N3	2.74 (5)	Eu6—Cl1	3.264 (8)
Eu2—C17 <sup>i</sup>	2.31 (6)	Eu6—O22 <sup>ii</sup>	2.369 (10)
Eu3—Cl1	3.227 (6)	Eu6—O23	2.412 (17)

Eu3—O19	2.373 (10)	Eu6—O5	2.46 (2)
Eu3—O17	2.368 (9)	O17—Eu3—O18	142.1 (3)
O19—Eu1—O20	73.4 (5)	O17 <sup>ii</sup> —Eu3—O11 <sup>iii</sup>	70.7 (5)
O19—Eu1—O18	73.0 (5)	O17 <sup>ii</sup> —Eu3—O11	134.7 (5)
O19—Eu1—O2W	71.6 (5)	O17—Eu3—O16	72.2 (5)
O19—Eu1—O9	149.6 (5)	O18—Eu3—Cl1	129.5 (4)
O19—Eu1—O10	62.8 (3)	O18—Eu3—O11 <sup>iii</sup>	71.7 (5)
O19—Eu1—O11	61.8 (4)	O18—Eu3—O16	100.6 (5)
O19—Eu1—O8	142.5 (5)	O11 <sup>iii</sup> —Eu3—Cl1	119.1 (4)
O19—Eu1—N2A	122.0 (10)	O11 <sup>iii</sup> —Eu3—O11	121.8 (8)
O19—Eu1—N2	122.4 (9)	O16—Eu3—Cl1	129.8 (4)
O20—Eu1—O2W	131.2 (5)	O16—Eu3—O11	72.1 (4)
O20—Eu1—O10	62.3 (5)	O19—Eu4—Cl1	66.9 (3)
O20—Eu1—O11	118.7 (5)	O19—Eu4—O19 <sup>iii</sup>	72.7 (5)
O20—Eu1—O8	135.5 (6)	O19 <sup>iii</sup> —Eu4—O22	134.3 (4)
O20—Eu1—N2A	127.9 (11)	O19—Eu4—O22	89.7 (4)
O20—Eu1—N2	72.6 (12)	O19—Eu4—O20	73.5 (4)
O18—Eu1—O20	66.1 (5)	O19—Eu4—O21	142.0 (3)
O18—Eu1—O2W	130.6 (6)	O19—Eu4—O10 <sup>iii</sup>	135.4 (5)
O18—Eu1—O9	82.6 (6)	O19 <sup>iii</sup> —Eu4—O10 <sup>iii</sup>	71.6 (4)
O18—Eu1—O10	118.8 (4)	O19 <sup>iii</sup> —Eu4—O10	135.4 (5)
O18—Eu1—O11	62.4 (5)	O22—Eu4—Cl1	67.4 (3)
O18—Eu1—O8	134.7 (6)	O22 <sup>iii</sup> —Eu4—O22	72.8 (5)
O18—Eu1—N2A	72.1 (11)	O22—Eu4—O20	142.0 (3)
O18—Eu1—N2	128.7 (14)	O22 <sup>iii</sup> —Eu4—O21	73.8 (4)
O2W—Eu1—O10	71.9 (5)	O22 <sup>iii</sup> —Eu4—O10 <sup>iii</sup>	71.0 (5)
O2W—Eu1—O11	70.9 (5)	O22—Eu4—O10 <sup>iii</sup>	134.7 (5)

O2W—Eu1—N2A	99.5 (11)	O20—Eu4—Cl1	130.2 (4)
O2W—Eu1—N2	99.3 (14)	O20—Eu4—O21	98.7 (6)
O9—Eu1—O20	80.4 (6)	O20—Eu4—O10	71.4 (4)
O9—Eu1—O2W	138.7 (6)	O21—Eu4—Cl1	131.2 (4)
O9—Eu1—O10	117.4 (5)	O21—Eu4—O10	70.7 (4)
O9—Eu1—O11	121.6 (5)	O10—Eu4—Cl1	119.9 (3)
O9—Eu1—O8	67.9 (6)	O10—Eu4—O10 <sup>iii</sup>	120.2 (7)
O9—Eu1—N2A	64.3 (10)	O22—Eu5—O23 <sup>ii</sup>	73.5 (5)
O9—Eu1—N2	61.3 (12)	O22—Eu5—O21	73.8 (4)
O11—Eu1—O10	120.1 (4)	O22—Eu5—O3W	71.9 (4)
O8—Eu1—O2W	70.9 (6)	O22—Eu5—O10	62.7 (4)
O8—Eu1—O10	105.4 (5)	O22—Eu5—O2	149.5 (5)
O8—Eu1—O11	104.6 (5)	O22—Eu5—O5	61.4 (5)
O8—Eu1—N2A	64.4 (11)	O22—Eu5—O3	142.9 (5)
O8—Eu1—N2	65.1 (11)	O22—Eu5—N1A	122.0 (9)
O17—Eu2—O1W	72.5 (7)	O22—Eu5—N1	121.6 (9)
O17—Eu2—O15	149.1 (7)	O23 <sup>ii</sup> —Eu5—O21	66.2 (5)
O17—Eu2—O11	61.4 (3)	O23 <sup>ii</sup> —Eu5—O3W	131.8 (5)
O17—Eu2—O16	72.8 (5)	O23 <sup>ii</sup> —Eu5—O10	119.0 (5)
O17—Eu2—O14	142.4 (7)	O23 <sup>ii</sup> —Eu5—O2	80.9 (6)
O1W—Eu2—O11	71.3 (4)	O23 <sup>ii</sup> —Eu5—O5	61.8 (6)
O1W—Eu2—O14	69.9 (8)	O23 <sup>ii</sup> —Eu5—O3	134.2 (6)
O1W—Eu2—N3	95.8 (11)	O23 <sup>ii</sup> —Eu5—N1A	129.7 (9)
O15—Eu2—O1W	138.3 (9)	O23 <sup>ii</sup> —Eu5—N1	72.2 (10)
O15—Eu2—O11 <sup>i</sup>	120.4 (3)	O21—Eu5—O3W	131.2 (5)
O15—Eu2—O14	68.4 (9)	O21—Eu5—O10	62.4 (4)
O15—Eu2—N3	64.9 (9)	O21—Eu5—O2	80.9 (5)

O11 <sup>i</sup> —Eu2—O11	118.2 (7)	O21—Eu5—O5	118.0 (6)
O16—Eu2—O1W	131.7 (5)	O21—Eu5—O3	134.8 (5)
O16 <sup>ii</sup> —Eu2—O15	81.3 (6)	O21—Eu5—N1A	73.2 (9)
O16 <sup>ii</sup> —Eu2—O11	117.8 (5)	O21—Eu5—N1	128.5 (10)
O16—Eu2—O11	62.9 (5)	O3W—Eu5—O10	71.5 (5)
O16 <sup>ii</sup> —Eu2—O16	65.0 (6)	O3W—Eu5—O5	72.5 (6)
O16 <sup>ii</sup> —Eu2—O14	135.7 (5)	O3W—Eu5—N1A	97.2 (9)
O16—Eu2—N3 <sup>i</sup>	131.2 (11)	O3W—Eu5—N1	99.0 (10)
O16 <sup>ii</sup> —Eu2—N3 <sup>i</sup>	75.6 (10)	O10—Eu5—O5	120.1 (5)
O14—Eu2—O11	105.4 (4)	O2—Eu5—O3W	138.6 (5)
O14—Eu2—N3	62.7 (9)	O2—Eu5—O10	119.3 (5)
N3—Eu2—O11	61.2 (8)	O2—Eu5—O5	119.6 (6)
N3 <sup>i</sup> —Eu2—O11	165.4 (11)	O2—Eu5—O3	67.6 (6)
N3—Eu2—N3 <sup>i</sup>	115.3 (15)	O2—Eu5—N1A	64.2 (10)
C17 <sup>i</sup> —Eu2—O17	103.7 (7)	O2—Eu5—N1	63.4 (10)
C17 <sup>i</sup> —Eu2—O1W	77.0 (14)	O3—Eu5—O3W	71.0 (5)
C17 <sup>i</sup> —Eu2—O15	87.5 (10)	O3—Eu5—O10	105.5 (5)
C17 <sup>i</sup> —Eu2—O11	147.8 (14)	O3—Eu5—O5	105.8 (6)
C17 <sup>i</sup> —Eu2—O11 <sup>i</sup>	42.7 (6)	O3—Eu5—N1A	64.3 (10)
C17 <sup>i</sup> —Eu2—O16 <sup>ii</sup>	79.6 (13)	O3—Eu5—N1	64.3 (10)
C17 <sup>i</sup> —Eu2—O16	144.0 (14)	N1A—Eu5—O10	59.9 (9)
C17 <sup>i</sup> —Eu2—O14	67.9 (9)	N1A—Eu5—O5	168.1 (10)
C17 <sup>i</sup> —Eu2—N3 <sup>i</sup>	22.7 (13)	N1—Eu5—O10	168.4 (10)
C17 <sup>i</sup> —Eu2—N3	129.3 (11)	N1—Eu5—O5	61.0 (10)
O19—Eu3—Cl1	66.6 (3)	N1—Eu5—N1A	116.4 (13)
O19 <sup>iii</sup> —Eu3—O19	73.0 (5)	O22—Eu6—Cl1	66.5 (2)
O19—Eu3—O18	73.4 (4)	O22—Eu6—O22 <sup>i</sup>	88.1 (5)

O19—Eu3—O11	70.7 (5)	O22—Eu6—O22 <sup>iii</sup>	73.5 (5)
O19 <sup>iii</sup> —Eu3—O11	135.2 (5)	O22—Eu6—O22 <sup>ii</sup>	133.0 (5)
O19 <sup>iii</sup> —Eu3—O11 <sup>iii</sup>	70.7 (5)	O22 <sup>ii</sup> —Eu6—O23	73.7 (4)
O19—Eu3—O16	142.3 (3)	O22 <sup>i</sup> —Eu6—O23 <sup>ii</sup>	142.1 (3)
O17—Eu3—Cl1	67.9 (3)	O22—Eu6—O23	142.1 (3)
O17 <sup>ii</sup> —Eu3—O19	134.5 (4)	O22 <sup>i</sup> —Eu6—O5 <sup>ii</sup>	135.8 (3)
O17—Eu3—O19	89.8 (4)	O22 <sup>i</sup> —Eu6—O5	71.2 (4)
O17 <sup>ii</sup> —Eu3—O17	72.6 (6)		

Symmetry codes: (i)  $-x+3/2, y, z$ ; (ii)  $-x+3/2, -y, z$ ; (iii)  $x, -y, z$ .

#### 4

Sm1—O1	2.429 (11)	Sm3—O18	2.507 (19)
Sm1—O1W	2.51 (2)	Sm3—O20	2.70 (4)
Sm1—N1	2.71 (5)	Sm4—O4	2.390 (14)
Sm1—O8	2.391 (15)	Sm4—O6	2.352 (13)
Sm1—O9	2.46 (3)	Sm4—O7	2.346 (12)
Sm1—O10	2.52 (3)	Sm4—O14A	2.57 (4)
Sm1—O14	2.65 (4)	Sm4—O20	2.57 (4)
Sm2—O2	2.40 (2)	Sm5—O5	2.428 (9)
Sm2—O7	2.345 (12)	Sm5—O6	2.395 (11)
Sm2—O8	2.355 (11)	Sm5—O14A	2.72 (4)
Sm2—O12	2.54 (4)	Sm5—O22	2.429 (15)
Sm2—O14	2.64 (4)	Sm5—O23	2.486 (17)
Sm3—O3	2.423 (9)	Sm6—O5 <sup>i</sup>	2.366 (17)
Sm3—O7	2.382 (12)	Sm6—O6 <sup>i</sup>	2.344 (11)
Sm3—O12	2.71 (3)	Sm6—O19A	2.57 (2)
Sm3—O17	2.452 (18)	O17—Sm3—O2W	138.4 (6)
O1 <sup>i</sup> —Sm1—O1	65.8 (8)	O17—Sm3—N2A	62.1 (10)

O1 <sup>i</sup> —Sm1—O1W	131.5 (5)	O17—Sm3—N2	63.1 (11)
O1 <sup>i</sup> —Sm1—N1	130.5 (13)	O17—Sm3—O12	119.1 (9)
O1—Sm1—N1	74.9 (13)	O17—Sm3—O18	67.6 (6)
O1 <sup>i</sup> —Sm1—O9	80.6 (11)	O17—Sm3—O20	118.3 (10)
O1—Sm1—O9	82.5 (11)	O18—Sm3—O2W	70.8 (6)
O1—Sm1—O10	135.0 (13)	O18—Sm3—N2A	66.7 (10)
O1 <sup>i</sup> —Sm1—O10	136.6 (15)	O18—Sm3—N2	63.0 (11)
O1 <sup>i</sup> —Sm1—O14	121.7 (10)	O18—Sm3—O12	102.0 (10)
O1 <sup>i</sup> —Sm1—O14 <sup>ii</sup>	65.2 (9)	O18—Sm3—O20	104.8 (10)
O1W—Sm1—N1	97.0 (13)	O3—Sm4—O4	100.3 (6)
O1W—Sm1—O10	69.2 (9)	O3—Sm4—O14A	76.5 (9)
O1W—Sm1—O14	69.5 (9)	O3—Sm4—O20	66.9 (9)
N1 <sup>ii</sup> —Sm1—N1	114 (2)	O4—Sm4—O14A	65.1 (8)
O8—Sm1—O1	72.7 (5)	O4—Sm4—O20	78.2 (8)
O8—Sm1—O1W	72.8 (7)	O6—Sm4—O3	143.3 (3)
O8—Sm1—N1	123.1 (10)	O6—Sm4—O4	74.2 (4)
O8—Sm1—O9	149.1 (9)	O6 <sup>iii</sup> —Sm4—O6	71.4 (6)
O8—Sm1—O10	142.1 (9)	O6 <sup>iii</sup> —Sm4—O14A	128.5 (9)
O8—Sm1—O14 <sup>ii</sup>	64.2 (9)	O6 <sup>iii</sup> —Sm4—O14A <sup>iii</sup>	68.2 (9)
O9—Sm1—O1W	137.9 (9)	O6—Sm4—O20	76.5 (9)
O9—Sm1—N1	65.0 (18)	O6—Sm4—O20 <sup>iii</sup>	142.1 (9)
O9—Sm1—N1 <sup>ii</sup>	61.9 (18)	O7—Sm4—O3	73.9 (5)
O9—Sm1—O10	68.8 (10)	O7—Sm4—O4	143.4 (3)
O10—Sm1—N1	62.0 (19)	O7 <sup>iii</sup> —Sm4—O6 <sup>iii</sup>	89.1 (4)
O10—Sm1—N1 <sup>ii</sup>	63.8 (19)	O7 <sup>iii</sup> —Sm4—O6	131.4 (4)
O14—Sm1—O14 <sup>ii</sup>	120.9 (18)	O7—Sm4—O7 <sup>iii</sup>	71.0 (6)
O1—Sm2—O2	100.9 (7)	O7 <sup>iii</sup> —Sm4—O14A	142.1 (9)

O1—Sm2—O12	77.1 (8)	O7—Sm4—O14A	78.5 (8)
O1—Sm2—O14	66.1 (8)	O7—Sm4—O20	66.2 (8)
O2—Sm2—O12	66.1 (8)	O7—Sm4—O20 <sup>iii</sup>	127.9 (8)
O2—Sm2—O14	79.6 (9)	O14A—Sm4—O14A <sup>iii</sup>	116.6 (17)
O7—Sm2—O1	143.4 (3)	O3W—Sm5—N3	99.8 (9)
O7—Sm2—O2	73.7 (5)	O3W—Sm5—N3A	98.1 (8)
O7 <sup>iii</sup> —Sm2—O7	71.0 (6)	O3W—Sm5—O14A	72.8 (9)
O7 <sup>iii</sup> —Sm2—O8 <sup>i</sup>	88.5 (5)	N3—Sm5—N3A	118.4 (11)
O7 <sup>iii</sup> —Sm2—O8	131.2 (5)	O4—Sm5—O3W	131.2 (5)
O7—Sm2—O8	88.5 (5)	O4—Sm5—N3	71.6 (9)
O7 <sup>iii</sup> —Sm2—O12	128.3 (8)	O4—Sm5—N3A	128.8 (8)
O7—Sm2—O12	67.6 (8)	O4—Sm5—O5	65.9 (5)
O7—Sm2—O14	77.4 (9)	O4—Sm5—O14A	62.4 (9)
O7—Sm2—O14 <sup>iii</sup>	143.1 (9)	O4—Sm5—O22	80.9 (5)
O8 <sup>i</sup> —Sm2—O1	74.4 (5)	O4—Sm5—O23	134.6 (6)
O8 <sup>i</sup> —Sm2—O2	143.0 (4)	O5—Sm5—O3W	130.1 (6)
O8 <sup>i</sup> —Sm2—O8	72.3 (8)	O5—Sm5—N3	128.4 (9)
O8—Sm2—O12 <sup>iii</sup>	142.6 (8)	O5—Sm5—N3A	72.3 (9)
O8 <sup>i</sup> —Sm2—O12 <sup>iii</sup>	77.2 (8)	O5—Sm5—O14A	120.1 (8)
O8—Sm2—O14	64.8 (10)	O5—Sm5—O22	80.2 (6)
O8—Sm2—O14 <sup>iii</sup>	127.4 (9)	O5—Sm5—O23	135.5 (6)
O12—Sm2—O12 <sup>iii</sup>	118.9 (17)	O6—Sm5—O3W	71.5 (5)
O14—Sm2—O14 <sup>iii</sup>	122.3 (17)	O6—Sm5—N3	120.6 (8)
O2W—Sm3—N2A	98.8 (11)	O6—Sm5—N3A	121.0 (8)
O2W—Sm3—N2	100.1 (11)	O6—Sm5—O4	72.9 (5)
O2W—Sm3—O12	72.1 (9)	O6—Sm5—O5	72.8 (5)
O2W—Sm3—O20	69.9 (9)	O6—Sm5—O14A	65.2 (8)

O2—Sm3—O2W	132.0 (6)	O6—Sm5—O22	148.1 (5)
O2—Sm3—N2A	127.7 (11)	O6—Sm5—O23	143.1 (6)
O2—Sm3—N2	72.6 (12)	O14A—Sm5—N3	56.6 (11)
O2—Sm3—O3	65.1 (5)	O14A—Sm5—N3A	167.4 (11)
O2—Sm3—O12	63.3 (9)	O22—Sm5—O3W	140.4 (6)
O2—Sm3—O17	81.8 (7)	O22—Sm5—N3	65.2 (9)
O2—Sm3—O18	133.7 (6)	O22—Sm5—N3A	63.8 (8)
O2—Sm3—O20	120.4 (10)	O22—Sm5—O14A	117.7 (9)
N2A—Sm3—N2	115.5 (13)	O22—Sm5—O23	68.8 (6)
O3—Sm3—O2W	131.0 (6)	O23—Sm5—O3W	71.6 (6)
O3—Sm3—N2A	72.5 (10)	O23—Sm5—N3	65.3 (10)
O3—Sm3—N2	127.6 (12)	O23—Sm5—N3A	65.8 (9)
O3—Sm3—O12	119.6 (10)	O23—Sm5—O14A	102.6 (9)
O3—Sm3—O17	81.1 (6)	O5 <sup>i</sup> —Sm6—O5	100.2 (8)
O3—Sm3—O18	136.7 (6)	O5—Sm6—O19A	77.9 (6)
O3—Sm3—O20	64.2 (9)	O5 <sup>i</sup> —Sm6—O19A	65.6 (6)
O7—Sm3—O2W	72.5 (5)	O6—Sm6—O5i	143.2 (3)
O7—Sm3—O2	72.9 (6)	O6—Sm6—O5	74.8 (4)
O7—Sm3—N2A	121.8 (9)	O6i—Sm6—O5	143.2 (3)
O7—Sm3—N2	122.7 (10)	O6—Sm6—O6ii	87.8 (6)
O7—Sm3—O3	72.5 (5)	O6—Sm6—O6iii	71.7 (6)
O7—Sm3—O12	64.3 (9)	O6—Sm6—O6i	130.3 (5)
O7—Sm3—O17	149.1 (6)	O6—Sm6—O19A	77.9 (7)
O7—Sm3—O18	143.3 (5)	O6ii—Sm6—O19A	66.8 (7)
O7—Sm3—O20	63.6 (10)	O6i—Sm6—O19A	128.2 (7)
O12—Sm3—N2A	167.7 (13)	O6iii—Sm6—O19A	143.3 (7)
O12—Sm3—N2	59.7 (13)		

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

<b>5</b>			
Ho1—O2	2.470 (8)	Ho5—O5	2.372 (7)
Ho1—O5	2.341 (7)	Ho5—O11	2.390 (8)
Ho1—O7	2.300 (6)	Ho5—O12	2.371 (7)
Ho1—O17	2.347 (7)	Ho5—O15	2.416 (7)
Ho2—Cl4	3.216 (7)	Ho5—O17 <sup>i</sup>	2.400 (7)
Ho2—O5	2.299 (6)	Ho5—O28	2.425 (10)
Ho2—O6	2.475 (7)	Ho6—N2 <sup>i</sup>	2.516 (12)
Ho2—O7	2.330 (6)	Ho6—O6 <sup>i</sup>	2.440 (7)
Ho2—O8	2.336 (7)	Ho6—O7 <sup>i</sup>	2.388 (6)
Ho2—O10	2.489 (7)	Ho6—O12 <sup>i</sup>	2.404 (6)
Ho2—O12	2.360 (7)	Ho6—O16	2.413 (8)
Ho2—O34	2.288 (7)	Ho6—O17	2.352 (7)
Ho3—O3 <sup>i</sup>	2.469 (7)	Ho6—O22 <sup>i</sup>	2.398 (10)
Ho3—Cl4	3.136 (17)	Ho6—O24 <sup>i</sup>	2.422 (9)
Ho3—O4	2.505 (7)	Ho7—O9	2.360 (7)
Ho3—O8	2.299 (7)	Ho7—O13	2.400 (8)
Ho3—O9	2.285 (6)	Ho7—O20	2.352 (7)
Ho3—O9 <sup>i</sup>	2.337 (7)	Ho7—O20 <sup>i</sup>	2.409 (7)
Ho3—O20	2.358 (7)	Ho7—O21	2.357 (9)
Ho3—O34	2.336 (7)	Ho7—O25	2.428 (10)
Ho3—O35	2.364 (7)	Ho8—O8	2.359 (7)
Ho4—O4	2.424 (8)	Ho8—O10	2.452 (7)
Ho4—O19	2.390 (8)	Ho8—O14	2.376 (11)
Ho4—O23	2.380 (8)	Ho8—O18 <sup>i</sup>	2.401 (8)
Ho4—O26	2.425 (8)	Ho8—O29	2.435 (10)

Ho4—O34	2.359 (6)	Ho8—O35	2.345 (7)
Ho4—O35	2.414 (7)	O11—Ho5—N4	66.4 (3)
O2 <sup>i</sup> —Ho1—O2	124.4 (3)	O11—Ho5—O15	86.4 (3)
O5—Ho1—O2 <sup>i</sup>	143.5 (2)	O11—Ho5—O17 <sup>i</sup>	80.5 (3)
O5—Ho1—O2	66.6 (2)	O11—Ho5—O28	70.7 (4)
O5 <sup>i</sup> —Ho1—O5	128.2 (3)	O12—Ho5—O2	123.8 (2)
O5—Ho1—O17	140.8 (2)	O12—Ho5—O3W	125.6 (3)
O5 <sup>i</sup> —Ho1—O17	76.6 (2)	O12—Ho5—N4	132.7 (3)
O7—Ho1—O2	127.8 (2)	O12—Ho5—O5	71.1 (2)
O7 <sup>i</sup> —Ho1—O2	78.5 (2)	O12—Ho5—O11	77.9 (2)
O7 <sup>i</sup> —Ho1—O5	87.1 (2)	O12—Ho5—O15	73.5 (2)
O7—Ho1—O5	70.3 (3)	O12—Ho5—O17 <sup>i</sup>	65.8 (2)
O7—Ho1—O7 <sup>i</sup>	127.3 (3)	O12—Ho5—O28	131.6 (4)
O7—Ho1—O17	148.1 (2)	O15—Ho5—O2	144.8 (2)
O7 <sup>i</sup> —Ho1—O17	72.7 (2)	O15—Ho5—O3W	73.4 (3)
O17 <sup>i</sup> —Ho1—O2	69.9 (2)	O15—Ho5—N4	130.7 (3)
O17—Ho1—O2	76.4 (2)	O15—Ho5—O28	68.8 (3)
O17 <sup>i</sup> —Ho1—O17	103.1 (4)	O17 <sup>i</sup> —Ho5—O2	69.1 (2)
O1—Ho2—Cl4	127.6 (4)	O17 <sup>i</sup> —Ho5—O3W	136.2 (3)
O1—Ho2—O6	77.2 (2)	O17 <sup>i</sup> —Ho5—N4	78.2 (3)
O1—Ho2—O10	68.3 (2)	O17 <sup>i</sup> —Ho5—O15	139.0 (2)
O1—Ho2—O12	101.0 (2)	O17 <sup>i</sup> —Ho5—O28	139.0 (3)
O5—Ho2—O1	146.2 (2)	O28—Ho5—O2	104.4 (4)
O5—Ho2—Cl4	66.6 (3)	O28—Ho5—O3W	70.1 (4)
O5—Ho2—O6	126.7 (2)	O28—Ho5—N4	63.9 (3)
O5—Ho2—O7	70.5 (3)	O2W—Ho6—N2 <sup>i</sup>	103.3 (4)
O5—Ho2—O8	88.6 (2)	O6 <sup>i</sup> —Ho6—O2W	72.3 (3)

O5—Ho2—O10	78.0 (2)	O6 <sup>i</sup> —Ho6—N2 <sup>i</sup>	64.0 (3)
O5—Ho2—O12	72.5 (2)	O7 <sup>i</sup> —Ho6—O2W	70.4 (3)
O6—Ho2—O10	123.8 (2)	O7 <sup>i</sup> —Ho6—N2 <sup>i</sup>	129.0 (3)
O7—Ho2—O1	141.8 (2)	O7 <sup>i</sup> —Ho6—O6 <sup>i</sup>	66.2 (2)
O7—Ho2—O6	66.5 (2)	O7 <sup>i</sup> —Ho6—O12 <sup>i</sup>	74.9 (2)
O7—Ho2—O8	129.4 (2)	O7 <sup>i</sup> —Ho6—O16	97.1 (2)
O7—Ho2—O10	143.4 (2)	O7 <sup>i</sup> —Ho6—O22 <sup>i</sup>	147.4 (3)
O7—Ho2—O12	76.8 (2)	O7 <sup>i</sup> —Ho6—O24 <sup>i</sup>	140.2 (3)
O8—Ho2—O1	75.8 (2)	O12 <sup>i</sup> —Ho6—O2W	135.3 (3)
O8—Ho2—O6	143.7 (2)	O12 <sup>i</sup> —Ho6—N2 <sup>i</sup>	77.7 (3)
O8—Ho2—O10	66.1 (2)	O12 <sup>i</sup> —Ho6—O6 <sup>i</sup>	68.3 (2)
O8—Ho2—O12	140.8 (2)	O12 <sup>i</sup> —Ho6—O16	139.8 (2)
O12—Ho2—Cl4	131.3 (4)	O12 <sup>i</sup> —Ho6—O24 <sup>i</sup>	138.5 (3)
O10—Ho2—Cl4	117.95 (18)	O16—Ho6—O2W	72.9 (3)
O12—Ho2—O6	68.4 (2)	O16—Ho6—N2 <sup>i</sup>	130.4 (3)
O12—Ho2—O10	76.3 (2)	O16—Ho6—O6 <sup>i</sup>	144.8 (2)
O34—Ho2—O1	72.4 (2)	O16—Ho6—O24 <sup>i</sup>	70.3 (3)
O34—Ho2—Cl4	63.9 (3)	O17—Ho6—O2W	124.6 (3)
O34—Ho2—O5	130.5 (2)	O17—Ho6—N2 <sup>i</sup>	132.0 (3)
O34—Ho2—O6	78.5 (2)	O17—Ho6—O6 <sup>i</sup>	123.4 (2)
O34—Ho2—O7	88.7 (2)	O17—Ho6—O7 <sup>i</sup>	71.1 (2)
O34—Ho2—O8	70.4 (3)	O17—Ho6—O12 <sup>i</sup>	66.1 (2)
O34—Ho2—O10	126.7 (2)	O17—Ho6—O16	74.0 (3)
O34—Ho2—O12	146.9 (2)	O17—Ho6—O22 <sup>i</sup>	78.5 (3)
O3 <sup>i</sup> —Ho3—Cl4	118.20 (17)	O17—Ho6—O24 <sup>i</sup>	134.3 (3)
O3 <sup>i</sup> —Ho3—O4	123.2 (2)	O22 <sup>i</sup> —Ho6—O2W	139.8 (3)
O4—Ho3—Cl4	118.58 (17)	O22 <sup>i</sup> —Ho6—N2 <sup>i</sup>	65.9 (4)

O8—Ho3—O3 <sup>i</sup>	78.9 (3)	O22 <sup>i</sup> —Ho6—O6 <sup>i</sup>	125.8 (3)
O8—Ho3—Cl4	65.6 (2)	O22 <sup>i</sup> —Ho6—O12 <sup>i</sup>	82.3 (3)
O8—Ho3—O4	126.3 (2)	O22 <sup>i</sup> —Ho6—O16	85.4 (3)
O8—Ho3—O9 <sup>i</sup>	89.7 (2)	O22 <sup>i</sup> —Ho6—O24 <sup>i</sup>	71.2 (3)
O8—Ho3—O20	147.4 (2)	O24 <sup>i</sup> —Ho6—O2W	69.8 (3)
O8—Ho3—O34	70.2 (3)	O24 <sup>i</sup> —Ho6—N2 <sup>i</sup>	62.7 (4)
O9—Ho3—O3 <sup>i</sup>	126.8 (2)	O24 <sup>i</sup> —Ho6—O6 <sup>i</sup>	102.1 (3)
O9 <sup>i</sup> —Ho3—O3 <sup>i</sup>	66.1 (2)	O3—Ho7—N5	63.3 (3)
O9 <sup>i</sup> —Ho3—Cl4	64.9 (2)	O5W—Ho7—O3	72.2 (3)
O9—Ho3—Cl4	65.4 (2)	O5W—Ho7—N5	100.0 (3)
O9 <sup>i</sup> —Ho3—O4	143.1 (2)	O5W—Ho7—O25	69.6 (4)
O9—Ho3—O4	77.9 (2)	O9—Ho7—O3	65.7 (2)
O9—Ho3—O8	131.0 (2)	O9—Ho7—O5W	72.2 (3)
O9—Ho3—O9 <sup>i</sup>	70.9 (3)	O9—Ho7—N5	128.2 (3)
O9 <sup>i</sup> —Ho3—O20	75.8 (2)	O9—Ho7—O13	97.4 (2)
O9—Ho3—O20	71.8 (2)	O9—Ho7—O20 <sup>i</sup>	74.4 (2)
O9—Ho3—O34	88.2 (2)	O9—Ho7—O25	141.6 (4)
O9 <sup>i</sup> —Ho3—O35	141.5 (2)	O13—Ho7—O3	145.6 (3)
O9—Ho3—O35	145.9 (2)	O13—Ho7—O5W	74.1 (3)
O20—Ho3—O3 <sup>i</sup>	68.6 (2)	O13—Ho7—N5	130.6 (3)
O20—Ho3—Cl4	128.8 (3)	O13—Ho7—O20 <sup>i</sup>	139.2 (3)
O20—Ho3—O4	76.1 (2)	O13—Ho7—O25	68.8 (3)
O20—Ho3—O35	101.5 (3)	O20 <sup>i</sup> —Ho7—O3	67.8 (2)
O34—Ho3—O3 <sup>i</sup>	144.0 (2)	O20—Ho7—O3	122.6 (2)
O34—Ho3—Cl4	65.0 (2)	O20 <sup>i</sup> —Ho7—O5W	135.6 (3)
O34—Ho3—O4	66.5 (2)	O20—Ho7—O5W	126.1 (3)
O34—Ho3—O9 <sup>i</sup>	129.9 (2)	O20 <sup>i</sup> —Ho7—N5	78.6 (3)

O34—Ho3—O20	140.6 (2)	O20—Ho7—N5	133.7 (3)
O34—Ho3—O35	76.2 (2)	O20—Ho7—O9	70.6 (2)
O35—Ho3—O3 <sup>i</sup>	77.1 (2)	O20—Ho7—O13	73.5 (3)
O35—Ho3—Cl4	129.6 (3)	O20—Ho7—O20 <sup>i</sup>	66.0 (3)
O35—Ho3—O4	68.1 (2)	O20—Ho7—O21	79.1 (3)
O1W—Ho4—N1	104.2 (3)	O20 <sup>i</sup> —Ho7—O25	139.2 (3)
O1—Ho4—O1W	125.6 (3)	O20—Ho7—O25	132.2 (4)
O1—Ho4—N1	130.0 (3)	O21—Ho7—O3	124.2 (3)
O1—Ho4—O4	123.6 (2)	O21—Ho7—O5W	139.8 (4)
O1—Ho4—O19	74.8 (3)	O21—Ho7—N5	66.1 (3)
O1—Ho4—O23	77.8 (3)	O21—Ho7—O9	146.6 (3)
O1—Ho4—O26	136.1 (3)	O21—Ho7—O13	86.9 (3)
O1—Ho4—O35	65.1 (2)	O21—Ho7—O20 <sup>i</sup>	80.8 (3)
O4—Ho4—O1W	72.1 (3)	O21—Ho7—O25	70.6 (4)
O4—Ho4—N1	64.8 (3)	O25—Ho7—O3	105.1 (3)
O4—Ho4—O26	100.2 (3)	O25—Ho7—N5	63.5 (3)
O19—Ho4—O1W	73.6 (3)	O1—Ho8—N3	78.6 (3)
O19—Ho4—N1	129.1 (3)	O1—Ho8—O4W	135.2 (3)
O19—Ho4—O4	145.5 (2)	O1—Ho8—O10	68.1 (3)
O19—Ho4—O26	70.5 (3)	O1—Ho8—O18 <sup>i</sup>	140.0 (3)
O19—Ho4—O35	139.6 (3)	O1—Ho8—O29	139.6 (3)
O23—Ho4—O1W	137.6 (3)	O4W—Ho8—N3	101.0 (3)
O23—Ho4—N1	66.5 (4)	O4W—Ho8—O10	71.7 (3)
O23—Ho4—O4	128.3 (3)	O8—Ho8—O1	74.4 (2)
O23—Ho4—O19	81.4 (4)	O8—Ho8—N3	129.4 (3)
O23—Ho4—O26	71.2 (3)	O8—Ho8—O4W	72.0 (3)
O23—Ho4—O35	85.1 (3)	O8—Ho8—O10	66.4 (2)

O26—Ho4—O1W	68.4 (3)	O8—Ho8—O14	147.3 (3)
O26—Ho4—N1	62.4 (3)	O8—Ho8—O18 <sup>i</sup>	96.9 (2)
O34—Ho4—O1W	70.9 (3)	O8—Ho8—O29	141.9 (3)
O34—Ho4—O1	70.5 (2)	O10—Ho8—N3	64.0 (3)
O34—Ho4—N1	130.9 (3)	O14—Ho8—O1	82.6 (3)
O34—Ho4—O4	67.5 (2)	O14—Ho8—N3	65.8 (4)
O34—Ho4—O19	97.4 (2)	O14—Ho8—O4W	138.7 (4)
O34—Ho4—O23	147.4 (3)	O14—Ho8—O10	125.5 (3)
O34—Ho4—O26	139.3 (3)	O14—Ho8—O18 <sup>i</sup>	85.9 (3)
O34—Ho4—O35	74.8 (2)	O14—Ho8—O29	69.0 (4)
O35—Ho4—N1	77.7 (3)	O18 <sup>i</sup> —Ho8—N3	130.0 (3)
O35—Ho4—O4	68.7 (2)	O18 <sup>i</sup> —Ho8—O4W	73.3 (3)
O35—Ho4—O26	139.0 (2)	O18 <sup>i</sup> —Ho8—O10	144.4 (3)
O2—Ho5—N4	63.5 (3)	O18 <sup>i</sup> —Ho8—O29	67.7 (3)
O3W—Ho5—O2	71.9 (3)	O29—Ho8—N3	64.0 (3)
O3W—Ho5—N4	101.6 (3)	O29—Ho8—O4W	70.2 (4)
O5—Ho5—O2	66.3 (2)	O29—Ho8—O10	105.4 (3)
O5—Ho5—O3W	71.6 (3)	O35—Ho8—O1	65.9 (2)
O5—Ho5—N4	128.7 (3)	O35—Ho8—N3	132.1 (3)
O5—Ho5—O11	146.3 (3)	O35—Ho8—O4W	126.7 (3)
O5—Ho5—O15	97.0 (2)	O35—Ho8—O8	71.3 (2)
O5—Ho5—O17 <sup>i</sup>	75.0 (2)	O35—Ho8—O10	123.7 (2)
O5—Ho5—O28	141.5 (4)	O35—Ho8—O14	78.3 (3)
O11—Ho5—O2	125.2 (3)	O35—Ho8—O18 <sup>i</sup>	74.3 (3)
O11—Ho5—O3W	140.2 (3)	O35—Ho8—O29	130.6 (4)
Symmetry code: (i) $x, -y+1/2, -z+1$ .			