

# Bis(2,2'-bipyridine- $\kappa^2N,N'$ )tris(nitrato- $\kappa^2O,O'$ )erbium(III)

Hua Yang

College of Chemistry and Chemical Engineering, Yan'an University, Yan'an, Shaanxi 716000, People's Republic of China

Correspondence e-mail: Yanghua7687@163.com

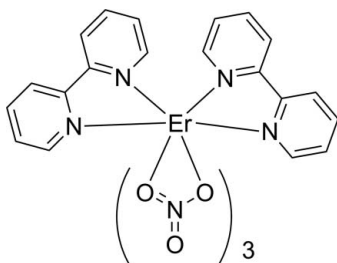
Received 16 March 2012; accepted 31 March 2012

 Key indicators: single-crystal X-ray study;  $T = 296$  K; mean  $\sigma(C-C) = 0.007$  Å;  $R$  factor = 0.018;  $wR$  factor = 0.051; data-to-parameter ratio = 16.9.

The asymmetric unit of the title compound,  $[Er(NO_3)_3 \cdot (C_{10}H_8N_2)_2]$ , contains one-half molecule situated on a twofold rotation axis. The  $Er^{III}$  ion is in a tenfold coordination by six O atoms from three  $NO_3^-$  anions and four N atoms from two 2,2'-bipyridine ligands in a distorted bicapped dodecahedral geometry. In the crystal, weak  $C-H \cdots O$  hydrogen bonds hold the molecules together.

## Related literature

For the crystal structures of related erbium complexes with 2,2'-bipyridine, see: Lu *et al.* (1995); Su *et al.* (1996); Staveren *et al.* (2000); Roh *et al.* (2005); Estrader *et al.* (2006); Ren *et al.* (2006). For potential applications of related complexes, see: Huskowska *et al.* (2002); Li *et al.* (2007); Puntus *et al.* (2009).



## Experimental

### Crystal data

 $[Er(NO_3)_3 \cdot (C_{10}H_8N_2)_2]$ 
 $M_r = 665.66$ 

 Orthorhombic, *Pbcn*
 $a = 16.5762$  (4) Å

 $b = 9.1158$  (2) Å

 $c = 15.0288$  (4) Å

 $V = 2270.93$  (10) Å<sup>3</sup>
 $Z = 4$ 

 Mo  $K\alpha$  radiation

 $\mu = 3.76$  mm<sup>-1</sup>
 $T = 296$  K

 $0.25 \times 0.23 \times 0.18$  mm

### Data collection

Bruker SMART CCD diffractometer

 Absorption correction: multi-scan (*SADABS*; Bruker, 2000)

 $T_{\min} = 0.453$ ,  $T_{\max} = 0.551$ 

11877 measured reflections

2859 independent reflections

 2127 reflections with  $I > 2\sigma(I)$ 
 $R_{\text{int}} = 0.016$ 

### Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.018$ 
 $wR(F^2) = 0.051$ 
 $S = 1.06$ 

2859 reflections

169 parameters

8 restraints

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 0.51$  e Å<sup>-3</sup>
 $\Delta\rho_{\text{min}} = -1.07$  e Å<sup>-3</sup>
**Table 1**

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$C5-H5 \cdots O6^i$	0.93	2.45	3.325 (6)	157
$C7-H7 \cdots O4^{ii}$	0.93	2.49	3.274 (6)	142

 Symmetry codes: (i)  $x + \frac{1}{2}, y - \frac{1}{2}, -z + \frac{1}{2}$ ; (ii)  $x + \frac{1}{2}, -y + \frac{3}{2}, -z + 1$ .

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The author appreciates financial support from Yanan University (grant No. YD2011–20) and the Science and Technology Bureau of Yanan City (grant No. kn2009–16).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV5264).

## References

- Bruker (2000). *SADABS*, *SAINT* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Estrader, M., Ribas, J., Tangoulis, V., Solans, X., Font-Bardia, M., Maestro, M. & Diaz, C. (2006). *Inorg. Chem.* **45**, 8239–8250.
- Huskowska, E., Turowska-Tyrk, I., Legendziewicz, J. & Riehl, J. P. (2002). *New J. Chem.* **26**, 1461–1467.
- Li, X., Zhang, T. T., Zhang, Z. Y. & Ju, Y. L. (2007). *J. Coord. Chem.* **60**, 2721–2729.
- Lu, W. M., Cheng, Y. Q., Dong, N., Gu, J. M. & Chen, C. G. (1995). *J. Coord. Chem.* **35**, 51–59.
- Puntus, L. N., Lyssenko, K. A., Pekareva, I. S. & Bunzli, J. G. (2009). *J. Phys. Chem. B*, **113**, 9265–9277.
- Ren, Y. X., Chen, S. P., Xie, G., Gao, S. L. & Shi, Q. Z. (2006). *Inorg. Chim. Acta*, **359**, 2047–2052.
- Roh, S. G., Nah, M. K., Oh, J. B., Baek, N. S., Park, K. M. & Kim, H. (2005). *Polyhedron*, **24**, 137–142.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Staveren, D. R. V., Hasnoot, J. G., Lanfredi, A. M. M., Menzer, S., Nieuwenhuizen, P. J., Spek, A. L., Ugozzoli, F. & Reedijk, J. (2000). *Inorg. Chim. Acta*, **307**, 81–87.
- Su, C. Y., Tang, N., Tan, M. Y. & Yu, K. B. (1996). *Polyhedron*, **15**, 233–239.

## supporting information

*Acta Cryst.* (2012). E68, m577 [doi:10.1107/S1600536812014031]

**Bis(2,2'-bipyridine- $\kappa^2N,N'$ )tris(nitrato- $\kappa^2O,O'$ )erbium(III)****Hua Yang****S1. Comment**

The synthesis and characterization of lanthanide complexes supported by *N,O*-chelating ligands and 2,2'-bipyridine have attracted continuous interest, due to the potential application of these compounds in magnetic, electronic and luminescent devices (Puntus *et al.*, 2009). Particularly, it was found that the coordination of 2,2'-bipyridine to the metal centers of the complexes could effectively tune the structures and properties of the resulting complexes (Li *et al.*, 2007; Huskowska *et al.*, 2002). Several erbium complexes with 2,2'-bipyridine have been reported (Staveren *et al.*, 2000; Su *et al.*, 1996; Lu *et al.*, 1995; Estrader *et al.*, 2006; Ren *et al.*, 2006; Roh *et al.*, 2005). In our attempts to synthesize the Er<sup>III</sup> complex supported by salicylaldehyde thiosemicarbazone and 2,2'-bipyridine, we obtained the title compound (I).

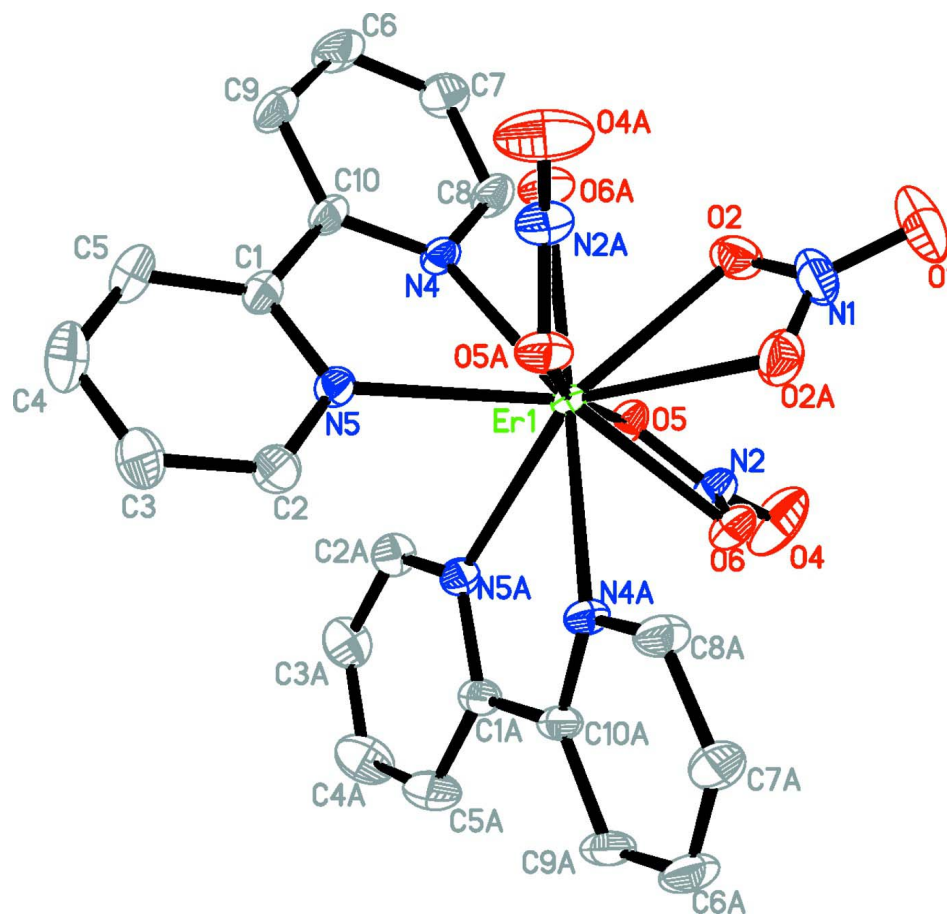
In (I) (Fig. 1), each NO<sub>3</sub><sup>-</sup> anion chelates to the metal center in a bidentate fashion. The central Er<sup>III</sup> ion adopts distorted bicapped dodecahedron geometry. The weak intermolecular C—H...O hydrogen bonds (Table 1) held the molecules together (Fig. 2).

**S2. Experimental**

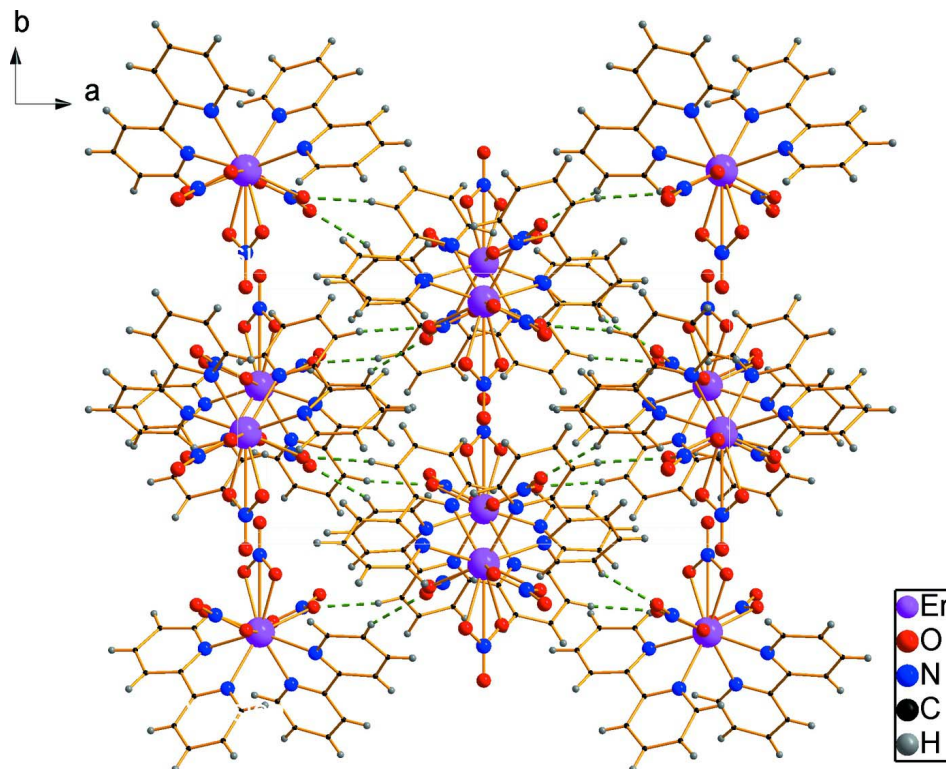
A mixture of Er(NO<sub>3</sub>)<sub>3</sub>·6H<sub>2</sub>O (0.0460 g, 0.1 mmol), 2,2'-bipyridine (0.0312 g, 0.2 mmol), salicylaldehyde thiosemicarbazone (0.0195 g, 0.1 mmol) and C<sub>2</sub>H<sub>5</sub>OH (3 ml) was sealed in a 6 ml Pyrex-tube. The tube was heated at 70 °C for 3 days under autogenous pressure. Cooling of the resultant solution to room temperature gave light pink crystals. The crystals were collected by filtration, washed with C<sub>2</sub>H<sub>5</sub>OH (2 ml) and dried in air.

**S3. Refinement**

H atoms were placed in calculated positions with C—H = 0.93 (aromatic and pyrrole) and refined in riding mode, with  $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$ .

**Figure 1**

The molecular structure of the title compound, with atom labels and 30% probability displacement ellipsoids [symmetry code: (A)  $-x, y, -z + 1/2$ ]. The H atoms have been omitted for clarity.

**Figure 2**

A portion of the crystal packing viewed down the  $c$ -axis. Hydrogen bonds are shown as dashed lines.

### Bis(2,2'-bipyridine- $\kappa^2N,N'$ )tris(nitrato- $\kappa^2O,O'$ )erbium(III)

#### Crystal data

[Er(NO<sub>3</sub>)<sub>3</sub>(C<sub>10</sub>H<sub>8</sub>N<sub>2</sub>)<sub>2</sub>]

$M_r = 665.66$

Orthorhombic, *Pbcn*

Hall symbol: -P 2n 2ab

$a = 16.5762$  (4) Å

$b = 9.1158$  (2) Å

$c = 15.0288$  (4) Å

$V = 2270.93$  (10) Å<sup>3</sup>

$Z = 4$

$F(000) = 1300$

$D_x = 1.947$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 5852 reflections

$\theta = 2.6$ – $26.5^\circ$

$\mu = 3.76$  mm<sup>-1</sup>

$T = 296$  K

Block, pink

$0.25 \times 0.23 \times 0.18$  mm

#### Data collection

Bruker SMART CCD  
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$\varphi$  scans and  $\omega$  scans

Absorption correction: multi-scan  
(*SADABS*; Bruker, 2000)

$T_{\min} = 0.453$ ,  $T_{\max} = 0.551$

11877 measured reflections

2859 independent reflections

2127 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.016$

$\theta_{\max} = 28.5^\circ$ ,  $\theta_{\min} = 2.5^\circ$

$h = -22 \rightarrow 22$

$k = -12 \rightarrow 7$

$l = -20 \rightarrow 15$

Refinement

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.018$   
 $wR(F^2) = 0.051$   
 $S = 1.06$   
 2859 reflections  
 169 parameters  
 8 restraints  
 Primary atom site location: structure-invariant  
 direct methods

Secondary atom site location: difference Fourier  
 map  
 Hydrogen site location: inferred from  
 neighbouring sites  
 H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0189P)^2 + 3.3713P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.010$   
 $\Delta\rho_{\max} = 0.51 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -1.07 \text{ e } \text{\AA}^{-3}$

Special details

**Geometry.** All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted  $R$ -factor  $wR$  and goodness of fit  $S$  are based on  $F^2$ , conventional  $R$ -factors  $R$  are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > \sigma(F^2)$  is used only for calculating  $R$ -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement.  $R$ -factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and  $R$ -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Er1	0.0000	0.59232 (2)	0.2500	0.02279 (8)
O1	0.0000	1.0374 (6)	0.2500	0.0790 (13)
O2	0.0381 (2)	0.8323 (4)	0.3082 (3)	0.0487 (8)
O4	-0.1240 (3)	0.7247 (6)	0.4738 (3)	0.0789 (15)
O5	-0.01985 (19)	0.6182 (4)	0.4172 (2)	0.0391 (8)
O6	-0.11602 (17)	0.6865 (4)	0.3319 (2)	0.0393 (7)
N1	0.0000	0.9058 (6)	0.2500	0.0535 (12)
N2	-0.0876 (2)	0.6777 (5)	0.4101 (3)	0.0411 (9)
N4	0.12765 (19)	0.5175 (4)	0.3252 (2)	0.0305 (8)
N5	0.0672 (2)	0.3730 (4)	0.1854 (2)	0.0295 (7)
C1	0.1431 (2)	0.3387 (5)	0.2090 (3)	0.0320 (9)
C2	0.0322 (3)	0.2940 (5)	0.1210 (3)	0.0386 (10)
H2	-0.0203	0.3175	0.1044	0.046*
C3	0.0699 (3)	0.1800 (6)	0.0783 (4)	0.0487 (12)
H3	0.0435	0.1277	0.0338	0.058*
C4	0.1470 (4)	0.1449 (7)	0.1025 (4)	0.0591 (15)
H4	0.1738	0.0676	0.0750	0.071*
C5	0.1845 (3)	0.2258 (6)	0.1683 (4)	0.0495 (13)
H5	0.2372	0.2043	0.1851	0.059*
C6	0.2890 (3)	0.5056 (6)	0.3713 (4)	0.0508 (13)
H6	0.3436	0.5042	0.3852	0.061*
C7	0.2369 (3)	0.5918 (6)	0.4189 (4)	0.0466 (13)
H7	0.2549	0.6468	0.4671	0.056*
C8	0.1569 (3)	0.5945 (5)	0.3933 (3)	0.0401 (11)
H8	0.1215	0.6534	0.4254	0.048*

C9	0.2597 (3)	0.4212 (6)	0.3027 (4)	0.0430 (12)
H9	0.2941	0.3599	0.2709	0.052*
C10	0.1788 (2)	0.4283 (5)	0.2813 (3)	0.0312 (9)

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Er1	0.01451 (11)	0.02538 (13)	0.02849 (13)	0.000	-0.00210 (10)	0.000
O1	0.130 (4)	0.030 (2)	0.077 (3)	0.000	0.029 (2)	0.000
O2	0.0448 (19)	0.0446 (19)	0.057 (2)	-0.0123 (16)	0.0024 (16)	-0.0140 (16)
O4	0.061 (3)	0.131 (4)	0.045 (2)	0.038 (3)	0.012 (2)	-0.023 (3)
O5	0.0302 (15)	0.0477 (19)	0.0395 (18)	0.0095 (13)	-0.0062 (13)	-0.0049 (15)
O6	0.0268 (15)	0.052 (2)	0.0386 (18)	0.0071 (14)	-0.0040 (13)	-0.0030 (15)
N1	0.068 (4)	0.027 (2)	0.066 (3)	0.000	0.027 (2)	0.000
N2	0.0324 (19)	0.052 (2)	0.039 (2)	0.0068 (18)	0.0021 (17)	-0.0051 (19)
N4	0.0216 (15)	0.0360 (19)	0.034 (2)	0.0031 (14)	-0.0041 (14)	-0.0003 (16)
N5	0.0270 (17)	0.0315 (18)	0.0299 (18)	0.0010 (14)	0.0023 (14)	-0.0008 (15)
C1	0.029 (2)	0.034 (2)	0.033 (2)	0.0056 (17)	0.0025 (18)	0.0036 (19)
C2	0.038 (2)	0.040 (2)	0.037 (2)	0.000 (2)	-0.001 (2)	-0.002 (2)
C3	0.062 (3)	0.044 (3)	0.040 (3)	0.002 (2)	0.001 (2)	-0.011 (2)
C4	0.071 (4)	0.053 (3)	0.053 (4)	0.022 (3)	0.007 (3)	-0.014 (3)
C5	0.042 (3)	0.056 (3)	0.051 (3)	0.020 (2)	0.005 (2)	-0.003 (3)
C6	0.024 (2)	0.065 (3)	0.064 (4)	0.004 (2)	-0.013 (2)	0.009 (3)
C7	0.036 (3)	0.052 (3)	0.051 (3)	-0.001 (2)	-0.019 (2)	-0.002 (2)
C8	0.029 (2)	0.049 (3)	0.042 (3)	0.0061 (19)	-0.0081 (19)	-0.008 (2)
C9	0.025 (2)	0.051 (3)	0.053 (3)	0.0123 (19)	-0.002 (2)	0.004 (2)
C10	0.0232 (19)	0.036 (2)	0.034 (2)	0.0068 (16)	0.0002 (17)	0.0059 (18)

*Geometric parameters (Å, °)*

Er1—O2 <sup>i</sup>	2.439 (3)	N5—C1	1.345 (5)
Er1—O2	2.439 (3)	C1—C5	1.380 (6)
Er1—O6	2.439 (3)	C1—C10	1.482 (7)
Er1—O6 <sup>i</sup>	2.439 (3)	C2—C3	1.372 (7)
Er1—N5	2.486 (3)	C2—H2	0.9300
Er1—N5 <sup>i</sup>	2.486 (3)	C3—C4	1.367 (8)
Er1—N4 <sup>i</sup>	2.494 (3)	C3—H3	0.9300
Er1—N4	2.494 (3)	C4—C5	1.382 (8)
Er1—O5 <sup>i</sup>	2.544 (3)	C4—H4	0.9300
Er1—O5	2.544 (3)	C5—H5	0.9300
O1—N1	1.199 (8)	C6—C7	1.369 (8)
O2—N1	1.270 (5)	C6—C9	1.375 (8)
O4—N2	1.210 (5)	C6—H6	0.9300
O5—N2	1.251 (5)	C7—C8	1.381 (6)
O6—N2	1.270 (5)	C7—H7	0.9300
N1—O2 <sup>i</sup>	1.270 (5)	C8—H8	0.9300
N4—C8	1.333 (6)	C9—C10	1.381 (6)
N4—C10	1.347 (5)	C9—H9	0.9300

N5—C2	1.339 (6)		
O2 <sup>i</sup> —Er1—O2	52.50 (19)	N2—O5—Er1	94.2 (3)
O2 <sup>i</sup> —Er1—O6	70.17 (12)	N2—O6—Er1	98.8 (2)
O2—Er1—O6	73.01 (12)	O1—N1—O2 <sup>i</sup>	121.9 (3)
O2 <sup>i</sup> —Er1—O6 <sup>i</sup>	73.01 (12)	O1—N1—O2	121.9 (3)
O2—Er1—O6 <sup>i</sup>	70.17 (12)	O2 <sup>i</sup> —N1—O2	116.2 (5)
O6—Er1—O6 <sup>i</sup>	138.78 (17)	O4—N2—O5	122.3 (4)
O2 <sup>i</sup> —Er1—N5	134.21 (13)	O4—N2—O6	121.7 (4)
O2—Er1—N5	138.18 (12)	O5—N2—O6	116.0 (4)
O6—Er1—N5	146.44 (11)	C8—N4—C10	117.7 (4)
O6 <sup>i</sup> —Er1—N5	74.51 (11)	C8—N4—Er1	120.8 (3)
O2 <sup>i</sup> —Er1—N5 <sup>i</sup>	138.18 (12)	C10—N4—Er1	118.5 (3)
O2—Er1—N5 <sup>i</sup>	134.21 (13)	C2—N5—C1	118.1 (4)
O6—Er1—N5 <sup>i</sup>	74.51 (12)	C2—N5—Er1	121.4 (3)
O6 <sup>i</sup> —Er1—N5 <sup>i</sup>	146.44 (11)	C1—N5—Er1	120.2 (3)
N5—Er1—N5 <sup>i</sup>	72.93 (16)	N5—C1—C5	121.5 (4)
O2 <sup>i</sup> —Er1—N4 <sup>i</sup>	82.13 (12)	N5—C1—C10	116.0 (4)
O2—Er1—N4 <sup>i</sup>	128.87 (12)	C5—C1—C10	122.5 (4)
O6—Er1—N4 <sup>i</sup>	69.87 (11)	N5—C2—C3	123.3 (5)
O6 <sup>i</sup> —Er1—N4 <sup>i</sup>	122.46 (11)	N5—C2—H2	118.4
N5—Er1—N4 <sup>i</sup>	89.02 (11)	C3—C2—H2	118.4
N5 <sup>i</sup> —Er1—N4 <sup>i</sup>	64.99 (12)	C4—C3—C2	118.6 (5)
O2 <sup>i</sup> —Er1—N4	128.87 (12)	C4—C3—H3	120.7
O2—Er1—N4	82.13 (12)	C2—C3—H3	120.7
O6—Er1—N4	122.46 (11)	C3—C4—C5	119.1 (5)
O6 <sup>i</sup> —Er1—N4	69.87 (11)	C3—C4—H4	120.4
N5—Er1—N4	64.99 (12)	C5—C4—H4	120.4
N5 <sup>i</sup> —Er1—N4	89.02 (11)	C1—C5—C4	119.4 (5)
N4 <sup>i</sup> —Er1—N4	148.26 (17)	C1—C5—H5	120.3
O2 <sup>i</sup> —Er1—O5 <sup>i</sup>	66.21 (12)	C4—C5—H5	120.3
O2—Er1—O5 <sup>i</sup>	103.72 (12)	C7—C6—C9	119.4 (4)
O6—Er1—O5 <sup>i</sup>	124.56 (10)	C7—C6—H6	120.3
O6 <sup>i</sup> —Er1—O5 <sup>i</sup>	50.76 (10)	C9—C6—H6	120.3
N5—Er1—O5 <sup>i</sup>	68.33 (11)	C6—C7—C8	118.1 (5)
N5 <sup>i</sup> —Er1—O5 <sup>i</sup>	121.21 (11)	C6—C7—H7	121.0
N4 <sup>i</sup> —Er1—O5 <sup>i</sup>	71.80 (11)	C8—C7—H7	121.0
N4—Er1—O5 <sup>i</sup>	111.28 (11)	N4—C8—C7	123.6 (5)
O2 <sup>i</sup> —Er1—O5	103.72 (12)	N4—C8—H8	118.2
O2—Er1—O5	66.21 (12)	C7—C8—H8	118.2
O6—Er1—O5	50.76 (10)	C6—C9—C10	119.4 (5)
O6 <sup>i</sup> —Er1—O5	124.56 (10)	C6—C9—H9	120.3
N5—Er1—O5	121.21 (11)	C10—C9—H9	120.3
N5 <sup>i</sup> —Er1—O5	68.33 (11)	N4—C10—C9	121.7 (5)
N4 <sup>i</sup> —Er1—O5	111.28 (11)	N4—C10—C1	116.1 (4)
N4—Er1—O5	71.80 (11)	C9—C10—C1	122.2 (4)
O5 <sup>i</sup> —Er1—O5	169.37 (15)		

O2 <sup>i</sup> —Er1—O2—N1	0.001 (1)	O5 <sup>i</sup> —Er1—N4—C10	-33.6 (3)
O6—Er1—O2—N1	-77.72 (18)	O5—Er1—N4—C10	157.2 (3)
O6 <sup>i</sup> —Er1—O2—N1	83.41 (19)	N1—Er1—N4—C10	-124.0 (3)
N5—Er1—O2—N1	117.4 (2)	O2 <sup>i</sup> —Er1—N5—C2	-65.7 (4)
N5 <sup>i</sup> —Er1—O2—N1	-124.34 (19)	O2—Er1—N5—C2	-144.9 (3)
N4 <sup>i</sup> —Er1—O2—N1	-32.8 (3)	O6—Er1—N5—C2	61.9 (4)
N4—Er1—O2—N1	154.8 (2)	O6 <sup>i</sup> —Er1—N5—C2	-111.8 (4)
O5 <sup>i</sup> —Er1—O2—N1	44.7 (2)	N5 <sup>i</sup> —Er1—N5—C2	76.4 (3)
O5—Er1—O2—N1	-131.7 (2)	N4 <sup>i</sup> —Er1—N5—C2	12.3 (3)
O2 <sup>i</sup> —Er1—O5—N2	46.4 (3)	N4—Er1—N5—C2	173.5 (4)
O2—Er1—O5—N2	83.9 (3)	O5 <sup>i</sup> —Er1—N5—C2	-58.4 (3)
O6—Er1—O5—N2	-3.1 (2)	O5—Er1—N5—C2	126.8 (3)
O6 <sup>i</sup> —Er1—O5—N2	125.0 (3)	N1—Er1—N5—C2	-103.6 (3)
N5—Er1—O5—N2	-142.8 (3)	O2 <sup>i</sup> —Er1—N5—C1	108.3 (3)
N5 <sup>i</sup> —Er1—O5—N2	-90.4 (3)	O2—Er1—N5—C1	29.1 (4)
N4 <sup>i</sup> —Er1—O5—N2	-40.4 (3)	O6—Er1—N5—C1	-124.1 (3)
N4—Er1—O5—N2	173.2 (3)	O6 <sup>i</sup> —Er1—N5—C1	62.2 (3)
O5 <sup>i</sup> —Er1—O5—N2	64.6 (3)	N5 <sup>i</sup> —Er1—N5—C1	-109.6 (4)
O2 <sup>i</sup> —Er1—O6—N2	-125.3 (3)	N4 <sup>i</sup> —Er1—N5—C1	-173.7 (3)
O2—Er1—O6—N2	-69.8 (3)	N4—Er1—N5—C1	-12.5 (3)
O6 <sup>i</sup> —Er1—O6—N2	-97.3 (3)	O5 <sup>i</sup> —Er1—N5—C1	115.6 (3)
N5—Er1—O6—N2	91.9 (3)	O5—Er1—N5—C1	-59.2 (3)
N5 <sup>i</sup> —Er1—O6—N2	77.5 (3)	N1—Er1—N5—C1	70.4 (4)
N4 <sup>i</sup> —Er1—O6—N2	146.1 (3)	C2—N5—C1—C5	0.2 (7)
N4—Er1—O6—N2	-1.1 (3)	Er1—N5—C1—C5	-174.0 (4)
O5 <sup>i</sup> —Er1—O6—N2	-165.0 (3)	C2—N5—C1—C10	-179.3 (4)
O5—Er1—O6—N2	3.1 (2)	Er1—N5—C1—C10	6.5 (5)
Er1—O2—N1—O1	180.000 (1)	C1—N5—C2—C3	0.1 (7)
Er1—O2—N1—O2 <sup>i</sup>	-0.001 (1)	Er1—N5—C2—C3	174.3 (4)
Er1—O5—N2—O4	-174.6 (5)	N5—C2—C3—C4	0.0 (8)
Er1—O5—N2—O6	5.1 (4)	C2—C3—C4—C5	-0.5 (9)
Er1—O6—N2—O4	174.4 (5)	N5—C1—C5—C4	-0.7 (8)
Er1—O6—N2—O5	-5.4 (4)	C10—C1—C5—C4	178.8 (5)
O2 <sup>i</sup> —Er1—N4—C8	50.6 (4)	C3—C4—C5—C1	0.9 (9)
O2—Er1—N4—C8	24.8 (4)	C9—C6—C7—C8	-2.5 (8)
O6—Er1—N4—C8	-39.2 (4)	C10—N4—C8—C7	2.5 (7)
O6 <sup>i</sup> —Er1—N4—C8	96.5 (4)	Er1—N4—C8—C7	-157.8 (4)
N5—Er1—N4—C8	178.3 (4)	C6—C7—C8—N4	0.3 (8)
N5 <sup>i</sup> —Er1—N4—C8	-110.1 (4)	C7—C6—C9—C10	2.0 (8)
N4 <sup>i</sup> —Er1—N4—C8	-143.9 (4)	C8—N4—C10—C9	-3.1 (7)
O5 <sup>i</sup> —Er1—N4—C8	126.5 (3)	Er1—N4—C10—C9	157.7 (4)
O5—Er1—N4—C8	-42.6 (3)	C8—N4—C10—C1	176.9 (4)
N1—Er1—N4—C8	36.1 (4)	Er1—N4—C10—C1	-22.3 (5)
O2 <sup>i</sup> —Er1—N4—C10	-109.6 (3)	C6—C9—C10—N4	0.9 (8)
O2—Er1—N4—C10	-135.3 (3)	C6—C9—C10—C1	-179.1 (5)
O6—Er1—N4—C10	160.6 (3)	N5—C1—C10—N4	10.4 (6)
O6 <sup>i</sup> —Er1—N4—C10	-63.6 (3)	C5—C1—C10—N4	-169.1 (4)
N5—Er1—N4—C10	18.2 (3)	N5—C1—C10—C9	-169.6 (4)



N5 <sup>i</sup> —Er1—N4—C10	89.7 (3)	C5—C1—C10—C9	11.0 (7)
N4 <sup>i</sup> —Er1—N4—C10	56.0 (3)		

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

*Hydrogen-bond geometry (Å, °)*

<i>D—H...A</i>	<i>D—H</i>	<i>H...A</i>	<i>D...A</i>	<i>D—H...A</i>
C5—H5...O6 <sup>ii</sup>	0.93	2.45	3.325 (6)	157
C7—H7...O4 <sup>iii</sup>	0.93	2.49	3.274 (6)	142

Symmetry codes: (ii)  $x+1/2, y-1/2, -z+1/2$ ; (iii)  $x+1/2, -y+3/2, -z+1$ .