

[*N,N'*-Bis(3-methoxy-2-oxidobenzylidene)ethane-1,2-diaminium- κ^4 O,O',O'',O''']tris(nitrato- κ^2 O,O')-erbium(III)

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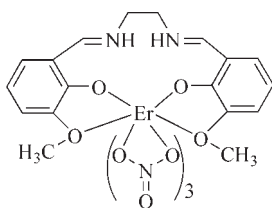
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Key indicators: single-crystal X-ray study; $T = 291$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.022; wR factor = 0.049; data-to-parameter ratio = 15.6.

In the mononuclear salen-type complex, $[\text{Er}(\text{NO}_3)_3(\text{C}_{18}\text{H}_{20}\text{N}_2\text{O}_4)]$, the Er^{III} ion is ten-coordinated in a distorted hexadecahedral geometry by six O atoms of three nitrate anions and four O atoms of the salen-like ligand. Intermolecular $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds occur. The crystal structure is stabilized by intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds.

Related literature

For similar lanthanide complexes of the same salen-like ligand, see: Gao *et al.* (2008, 2009).



Experimental

Crystal data

$[\text{Er}(\text{NO}_3)_3(\text{C}_{18}\text{H}_{20}\text{N}_2\text{O}_4)]$

$M_r = 681.65$

Monoclinic, $P2_1/n$

$a = 14.098$ (3) Å

$b = 11.865$ (2) Å

$c = 14.571$ (3) Å

$\beta = 103.98$ (3)°

$V = 2365.1$ (8) Å³

$Z = 4$

Mo $K\alpha$ radiation

$\mu = 3.63$ mm⁻¹

$T = 291$ K

$0.37 \times 0.36 \times 0.34$ mm

Data collection

Rigaku R-Axis RAPID

diffractometer

Absorption correction: multi-scan

(*ABSCOR*; Higashi, 1995)

$T_{\text{min}} = 0.344$, $T_{\text{max}} = 0.368$

21792 measured reflections

5358 independent reflections

4748 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.024$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.022$

$wR(F^2) = 0.049$

$S = 1.04$

5358 reflections

344 parameters

2 restraints

H atoms treated by a mixture of independent and constrained refinement

$\Delta\rho_{\text{max}} = 0.97$ e Å⁻³

$\Delta\rho_{\text{min}} = -0.32$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N}2-\text{H}2\cdots\text{O}3$	0.85 (1)	1.89 (3)	2.574 (3)	137 (3)
$\text{N}1-\text{H}1\cdots\text{O}1$	0.85 (1)	1.84 (2)	2.567 (3)	143 (3)
$\text{C}7-\text{H}7\cdots\text{O}5^{\text{i}}$	0.93	2.33	3.073 (3)	137
$\text{C}9-\text{H}9\text{A}\cdots\text{O}12^{\text{ii}}$	0.97	2.50	3.241 (3)	133
$\text{C}10-\text{H}10\cdots\text{O}9^{\text{iii}}$	0.93	2.57	3.395 (4)	148
$\text{C}14-\text{H}14\cdots\text{O}12^{\text{iv}}$	0.93	2.50	3.341 (4)	150

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalClear* (Rigaku/MSK, 2002); 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: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2218).

References

- Gao, T., Li, G.-M., Gao, P., Yan, P.-F. & Hou, G.-F. (2009). *Acta Cryst.* **E65**, m1585.
- Gao, T., Yan, P. F., Li, G. M., Hou, G. F. & Gao, J. S. (2008). *Inorg. Chim. Acta*, **361**, 2051–2058.
- Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
- Rigaku (1998). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.
- Rigaku/MSK (2002). *CrystalClear*. Rigaku/MSK Inc., The Woodlands, Texas, USA.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.

supplementary materials

Acta Cryst. (2010). E66, m107 [doi:10.1107/S1600536809055184]

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T. Gao, G.-M. Li, P. Gao, P.-F. Yan and G.-F. Hou

Comment

In continuation of our studies of salen-type lanthanide complexes (Gao *et al.*, 2008, 2009), we present here the crystal structure of the title compound. As shown in Fig. 1, the ten-coordinate Er^{III} ion adopts a hexadecahedral geometry provided by the O atoms of three bidentate nitrate anions and by one ligand that utilizes two hydroxyl and two methoxy oxygen atoms, while the protonated nitrogen atoms remain uncoordinated. This compound is isostructural with the corresponding Nd, Eu, Tb and Dy complexes (Gao *et al.*, 2008, 2009). The Er—O bond distances range from 2.2462 (19) to 2.682 (2) Å, with the shorter bonds involving the O1 and O3 deprotonated phenol oxygen atoms. The crystal structure is stabilized by intra- and intermolecular N—H \cdots O and C—H \cdots O hydrogen bonds (Table 1).

Experimental

The title complex was obtained by the treatment of erbium (III) nitrate hexahydrate (0.114 g, 0.25 mmol) with the salen-type ligand (0.083 g, 0.25 mmol) in acetonitrile/methanol (10 ml/10 ml). The mixture was stirred for 3 h. The reaction mixture was filtered; diethyl ether was allowed to diffuse slowly into the solution of the filtrate. Single crystals were obtained after several days. Analysis calculated for C₁₈H₂₀Er₁N₅O₁₃: C 31.72, H 2.96, N 10.27%; found: C 32.08, H 3.00, N 10.38%.

Refinement

H atoms bound to C atoms were placed in calculated positions and treated as riding on their parent atoms, with C—H = 0.93 Å (aromatic C), C—H = 0.97 Å (methylene C), and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or C—H = 0.96 Å (methyl C) and with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$. The N-bound H atoms were initially located in a difference Fourier map and they were refined with the N—H bond distance restrained to 0.85 Å.

Figures

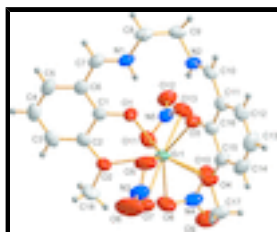


Fig. 1. The molecular structure of the the title compound, showing 30% probability displacement ellipsoids.

supplementary materials

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Hall symbol: -P 2yn

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$\beta = 103.98$ (3)°

$V = 2365.1$ (8) Å³

$Z = 4$

$F(000) = 1340$

$D_x = 1.914$ Mg m⁻³

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

Cell parameters from 19557 reflections

$\theta = 6.7$ – 55.0 °

$\mu = 3.63$ mm⁻¹

$T = 291$ K

Block, brown

$0.37 \times 0.36 \times 0.34$ mm

Data collection

Rigaku R-Axis RAPID
diffractometer

Radiation source: fine-focus sealed tube
graphite

Detector resolution: 10.000 pixels mm⁻¹

ω scans

Absorption correction: multi-scan
(*ABSCOR*; Higashi, 1995)

$T_{\min} = 0.344$, $T_{\max} = 0.368$

21792 measured reflections

5358 independent reflections

4748 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.024$

$\theta_{\max} = 27.5$ °, $\theta_{\min} = 3.4$ °

$h = -18 \rightarrow 18$

$k = -15 \rightarrow 13$

$l = -18 \rightarrow 18$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.022$

$wR(F^2) = 0.049$

$S = 1.04$

5358 reflections

344 parameters

2 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0212P)^2 + 1.495P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.002$

$\Delta\rho_{\max} = 0.97$ e Å⁻³

$\Delta\rho_{\min} = -0.32$ e Å⁻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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	1.11705 (18)	0.8605 (2)	0.45224 (18)	0.0382 (5)
C2	1.20341 (19)	0.8854 (2)	0.42275 (19)	0.0407 (5)
C3	1.28633 (19)	0.9208 (2)	0.4865 (2)	0.0473 (6)
H3	1.3434	0.9334	0.4667	0.057*
C4	1.2851 (2)	0.9379 (2)	0.5812 (2)	0.0514 (7)
H4	1.3416	0.9618	0.6241	0.062*
C5	1.2025 (2)	0.9199 (2)	0.6108 (2)	0.0482 (6)
H5	1.2021	0.9338	0.6736	0.058*
C6	1.11664 (18)	0.8802 (2)	0.54721 (17)	0.0398 (5)
C7	1.03136 (19)	0.8571 (2)	0.57937 (18)	0.0419 (6)
H7	1.0340	0.8661	0.6433	0.050*
C8	0.8585 (2)	0.8013 (2)	0.5501 (2)	0.0476 (6)
H8A	0.8190	0.8692	0.5424	0.057*
H8B	0.8721	0.7791	0.6161	0.057*
C9	0.8026 (2)	0.7084 (2)	0.4892 (2)	0.0463 (6)
H9A	0.8384	0.6381	0.5029	0.056*
H9B	0.7395	0.6985	0.5038	0.056*
C10	0.71313 (18)	0.7852 (2)	0.33653 (19)	0.0405 (6)
H10	0.6585	0.7963	0.3607	0.049*
C11	0.70956 (17)	0.8234 (2)	0.24387 (18)	0.0378 (5)
C12	0.62437 (19)	0.8736 (2)	0.1881 (2)	0.0487 (6)
H12	0.5690	0.8799	0.2118	0.058*
C13	0.6223 (2)	0.9123 (3)	0.1009 (2)	0.0562 (8)
H13	0.5652	0.9442	0.0647	0.067*
C14	0.7057 (2)	0.9052 (2)	0.0634 (2)	0.0509 (7)
H14	0.7033	0.9319	0.0029	0.061*
C15	0.78977 (18)	0.8588 (2)	0.11660 (18)	0.0393 (5)
C16	0.79432 (17)	0.8157 (2)	0.20754 (18)	0.0353 (5)
C17	0.8799 (3)	0.8857 (3)	-0.0015 (2)	0.0660 (9)
H15	0.8287	0.8495	-0.0475	0.099*
H16	0.9420	0.8669	-0.0135	0.099*
H17	0.8708	0.9659	-0.0056	0.099*
C18	1.2751 (3)	0.8925 (4)	0.2892 (3)	0.0813 (12)

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H18	1.2967	0.9685	0.3043	0.122*
H19	1.2567	0.8835	0.2217	0.122*
H20	1.3270	0.8411	0.3158	0.122*
Er1	1.027172 (8)	0.791612 (9)	0.235283 (7)	0.03487 (4)
H1	0.954 (2)	0.824 (3)	0.4667 (10)	0.055 (9)*
H2	0.8358 (18)	0.723 (3)	0.364 (2)	0.065 (10)*
N1	0.95017 (17)	0.8241 (2)	0.52382 (16)	0.0431 (5)
N2	0.78847 (16)	0.7357 (2)	0.38932 (16)	0.0410 (5)
N3	1.0155 (2)	1.0328 (2)	0.1988 (2)	0.0662 (7)
N4	1.07427 (19)	0.6872 (2)	0.07369 (18)	0.0498 (6)
N5	1.08572 (16)	0.57223 (19)	0.31635 (15)	0.0422 (5)
O1	1.04131 (13)	0.82028 (18)	0.39117 (13)	0.0500 (5)
O2	1.19230 (13)	0.86931 (18)	0.32755 (13)	0.0500 (5)
O3	0.87510 (12)	0.77016 (15)	0.25531 (12)	0.0393 (4)
O4	0.87710 (14)	0.84819 (17)	0.09111 (13)	0.0485 (4)
O5	0.97238 (19)	0.9849 (2)	0.25442 (16)	0.0729 (7)
O6	1.0101 (3)	1.1337 (2)	0.1861 (3)	0.1093 (11)
O7	1.06391 (17)	0.96856 (19)	0.15897 (16)	0.0613 (6)
O8	1.12293 (19)	0.7666 (2)	0.11639 (19)	0.0714 (7)
O9	1.0911 (2)	0.6461 (2)	0.00302 (18)	0.0794 (7)
O10	1.00528 (15)	0.6536 (2)	0.10706 (16)	0.0615 (6)
O11	1.14616 (13)	0.64176 (18)	0.29752 (16)	0.0543 (5)
O12	1.11095 (15)	0.48027 (17)	0.35168 (15)	0.0566 (5)
O13	0.99850 (14)	0.60343 (17)	0.29684 (16)	0.0547 (5)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0425 (13)	0.0366 (14)	0.0352 (13)	-0.0009 (10)	0.0089 (10)	0.0014 (10)
C2	0.0466 (14)	0.0346 (13)	0.0415 (14)	-0.0049 (10)	0.0119 (10)	-0.0005 (11)
C3	0.0432 (14)	0.0371 (14)	0.0607 (18)	-0.0041 (11)	0.0111 (12)	-0.0004 (13)
C4	0.0519 (16)	0.0423 (16)	0.0522 (17)	-0.0049 (12)	-0.0025 (12)	-0.0064 (13)
C5	0.0614 (17)	0.0391 (15)	0.0390 (15)	0.0005 (12)	0.0023 (12)	-0.0049 (11)
C6	0.0511 (14)	0.0329 (13)	0.0347 (13)	0.0027 (10)	0.0092 (10)	-0.0002 (10)
C7	0.0570 (16)	0.0376 (14)	0.0321 (13)	0.0075 (11)	0.0127 (11)	-0.0027 (10)
C8	0.0512 (15)	0.0602 (18)	0.0377 (14)	0.0090 (12)	0.0229 (11)	0.0051 (12)
C9	0.0495 (15)	0.0522 (16)	0.0425 (15)	0.0046 (11)	0.0217 (11)	0.0143 (12)
C10	0.0382 (13)	0.0407 (14)	0.0461 (15)	-0.0002 (10)	0.0170 (10)	-0.0042 (11)
C11	0.0364 (12)	0.0369 (13)	0.0406 (14)	0.0045 (9)	0.0102 (10)	-0.0024 (10)
C12	0.0402 (14)	0.0496 (16)	0.0546 (17)	0.0106 (11)	0.0084 (11)	-0.0028 (13)
C13	0.0496 (16)	0.0533 (18)	0.0577 (19)	0.0179 (13)	-0.0027 (13)	0.0056 (14)
C14	0.0638 (18)	0.0448 (16)	0.0390 (15)	0.0085 (12)	0.0022 (12)	0.0072 (12)
C15	0.0460 (14)	0.0371 (14)	0.0347 (13)	0.0039 (10)	0.0094 (10)	0.0018 (10)
C16	0.0378 (12)	0.0328 (13)	0.0353 (13)	0.0031 (9)	0.0091 (9)	0.0009 (9)
C17	0.081 (2)	0.084 (2)	0.0378 (16)	0.0008 (18)	0.0249 (15)	0.0118 (16)
C18	0.068 (2)	0.121 (3)	0.066 (2)	-0.041 (2)	0.0381 (18)	-0.012 (2)
Er1	0.03856 (7)	0.04067 (7)	0.02990 (6)	-0.00224 (4)	0.01707 (4)	0.00026 (4)
N1	0.0496 (13)	0.0531 (14)	0.0309 (12)	0.0030 (10)	0.0181 (9)	0.0011 (10)

N2	0.0410 (12)	0.0482 (13)	0.0382 (12)	0.0027 (9)	0.0183 (9)	0.0038 (9)
N3	0.107 (2)	0.0498 (17)	0.0492 (15)	-0.0087 (14)	0.0328 (15)	-0.0004 (13)
N4	0.0628 (15)	0.0502 (15)	0.0439 (13)	0.0119 (11)	0.0270 (11)	0.0006 (11)
N5	0.0452 (12)	0.0476 (13)	0.0352 (11)	0.0032 (9)	0.0124 (9)	0.0028 (9)
O1	0.0430 (10)	0.0761 (14)	0.0332 (10)	-0.0144 (9)	0.0136 (8)	-0.0086 (9)
O2	0.0476 (10)	0.0648 (13)	0.0430 (11)	-0.0166 (9)	0.0215 (8)	-0.0047 (9)
O3	0.0348 (9)	0.0484 (11)	0.0360 (9)	0.0081 (7)	0.0109 (7)	0.0099 (7)
O4	0.0574 (11)	0.0581 (12)	0.0335 (10)	0.0032 (9)	0.0179 (8)	0.0075 (8)
O5	0.127 (2)	0.0497 (14)	0.0611 (15)	-0.0098 (12)	0.0588 (15)	-0.0098 (10)
O6	0.192 (3)	0.0431 (16)	0.116 (3)	0.0054 (17)	0.082 (2)	0.0152 (16)
O7	0.0805 (15)	0.0568 (13)	0.0560 (13)	-0.0025 (11)	0.0344 (11)	0.0099 (11)
O8	0.0880 (17)	0.0701 (16)	0.0739 (17)	-0.0253 (13)	0.0539 (14)	-0.0199 (13)
O9	0.118 (2)	0.0705 (17)	0.0685 (16)	0.0085 (14)	0.0590 (15)	-0.0145 (13)
O10	0.0520 (12)	0.0793 (16)	0.0589 (14)	-0.0083 (10)	0.0245 (10)	-0.0197 (11)
O11	0.0397 (10)	0.0558 (13)	0.0686 (14)	-0.0013 (8)	0.0151 (9)	0.0030 (10)
O12	0.0679 (13)	0.0489 (12)	0.0524 (12)	0.0159 (9)	0.0132 (9)	0.0122 (10)
O13	0.0414 (10)	0.0518 (12)	0.0753 (14)	0.0058 (8)	0.0225 (9)	0.0181 (10)

Geometric parameters (Å, °)

C1—O1	1.304 (3)	C15—C16	1.407 (3)
C1—C6	1.405 (3)	C16—O3	1.300 (3)
C1—C2	1.417 (3)	C17—O4	1.430 (3)
C2—C3	1.371 (4)	C17—H15	0.9600
C2—O2	1.371 (3)	C17—H16	0.9600
C3—C4	1.399 (4)	C17—H17	0.9600
C3—H3	0.9300	C18—O2	1.437 (3)
C4—C5	1.354 (4)	C18—H18	0.9600
C4—H4	0.9300	C18—H19	0.9600
C5—C6	1.416 (4)	C18—H20	0.9600
C5—H5	0.9300	Er1—O3	2.2469 (17)
C6—C7	1.419 (4)	Er1—O1	2.2576 (19)
C7—N1	1.293 (3)	Er1—O10	2.447 (2)
C7—H7	0.9300	Er1—O5	2.458 (2)
C8—N1	1.460 (3)	Er1—O8	2.458 (2)
C8—C9	1.512 (4)	Er1—O11	2.462 (2)
C8—H8A	0.9700	Er1—O13	2.476 (2)
C8—H8B	0.9700	Er1—O7	2.488 (2)
C9—N2	1.457 (3)	Er1—O2	2.562 (2)
C9—H9A	0.9700	Er1—O4	2.682 (2)
C9—H9B	0.9700	Er1—N4	2.877 (2)
C10—N2	1.292 (3)	Er1—N5	2.895 (2)
C10—C11	1.413 (4)	N1—H1	0.846 (10)
C10—H10	0.9300	N2—H2	0.847 (10)
C11—C12	1.409 (4)	N3—O6	1.211 (4)
C11—C16	1.422 (3)	N3—O7	1.255 (3)
C12—C13	1.344 (4)	N3—O5	1.260 (3)
C12—H12	0.9300	N4—O9	1.213 (3)
C13—C14	1.413 (4)	N4—O8	1.241 (3)

supplementary materials

C13—H13	0.9300	N4—O10	1.253 (3)
C14—C15	1.365 (4)	N5—O12	1.222 (3)
C14—H14	0.9300	N5—O13	1.249 (3)
C15—O4	1.375 (3)	N5—O11	1.263 (3)
O1—C1—C6	122.4 (2)	O8—Er1—O13	108.19 (8)
O1—C1—C2	119.4 (2)	O11—Er1—O13	51.07 (6)
C6—C1—C2	118.2 (2)	O3—Er1—O7	117.50 (7)
C3—C2—O2	126.7 (2)	O1—Er1—O7	110.20 (8)
C3—C2—C1	120.9 (2)	O10—Er1—O7	103.00 (8)
O2—C2—C1	112.4 (2)	O5—Er1—O7	50.82 (7)
C2—C3—C4	120.1 (3)	O8—Er1—O7	65.02 (8)
C2—C3—H3	120.0	O11—Er1—O7	125.25 (7)
C4—C3—H3	120.0	O13—Er1—O7	173.13 (7)
C5—C4—C3	120.6 (3)	O3—Er1—O2	138.34 (6)
C5—C4—H4	119.7	O1—Er1—O2	64.51 (6)
C3—C4—H4	119.7	O10—Er1—O2	124.92 (7)
C4—C5—C6	120.6 (3)	O5—Er1—O2	82.83 (8)
C4—C5—H5	119.7	O8—Er1—O2	80.16 (8)
C6—C5—H5	119.7	O11—Er1—O2	67.34 (7)
C1—C6—C5	119.6 (2)	O13—Er1—O2	109.97 (7)
C1—C6—C7	119.9 (2)	O7—Er1—O2	70.74 (7)
C5—C6—C7	120.4 (2)	O3—Er1—O4	62.17 (6)
N1—C7—C6	123.0 (2)	O1—Er1—O4	127.71 (7)
N1—C7—H7	118.5	O10—Er1—O4	68.86 (7)
C6—C7—H7	118.5	O5—Er1—O4	69.22 (8)
N1—C8—C9	110.5 (2)	O8—Er1—O4	86.66 (8)
N1—C8—H8A	109.6	O11—Er1—O4	143.86 (7)
C9—C8—H8A	109.6	O13—Er1—O4	110.04 (7)
N1—C8—H8B	109.6	O7—Er1—O4	69.43 (7)
C9—C8—H8B	109.6	O2—Er1—O4	139.98 (7)
H8A—C8—H8B	108.1	O3—Er1—N4	118.27 (8)
N2—C9—C8	110.5 (2)	O1—Er1—N4	155.06 (7)
N2—C9—H9A	109.5	O10—Er1—N4	25.63 (7)
C8—C9—H9A	109.5	O5—Er1—N4	129.48 (7)
N2—C9—H9B	109.5	O8—Er1—N4	25.37 (7)
C8—C9—H9B	109.5	O11—Er1—N4	73.69 (7)
H9A—C9—H9B	108.1	O13—Er1—N4	89.91 (7)
N2—C10—C11	123.3 (2)	O7—Er1—N4	83.31 (7)
N2—C10—H10	118.4	O2—Er1—N4	102.96 (7)
C11—C10—H10	118.4	O4—Er1—N4	76.17 (7)
C12—C11—C10	121.0 (2)	O3—Er1—N5	91.84 (6)
C12—C11—C16	119.2 (2)	O1—Er1—N5	77.16 (7)
C10—C11—C16	119.7 (2)	O10—Er1—N5	71.38 (8)
C13—C12—C11	120.7 (3)	O5—Er1—N5	149.24 (7)
C13—C12—H12	119.7	O8—Er1—N5	91.62 (8)
C11—C12—H12	119.7	O11—Er1—N5	25.67 (6)
C12—C13—C14	121.0 (2)	O13—Er1—N5	25.39 (6)
C12—C13—H13	119.5	O7—Er1—N5	150.63 (7)
C14—C13—H13	119.5	O2—Er1—N5	88.63 (7)

C15—C14—C13	119.6 (3)	O4—Er1—N5	129.63 (6)
C15—C14—H14	120.2	N4—Er1—N5	81.22 (7)
C13—C14—H14	120.2	C7—N1—C8	126.7 (2)
C14—C15—O4	126.5 (2)	C7—N1—H1	111 (2)
C14—C15—C16	121.1 (2)	C8—N1—H1	122 (2)
O4—C15—C16	112.4 (2)	C10—N2—C9	126.2 (2)
O3—C16—C15	119.3 (2)	C10—N2—H2	116 (2)
O3—C16—C11	122.2 (2)	C9—N2—H2	117 (2)
C15—C16—C11	118.4 (2)	O6—N3—O7	123.4 (3)
O4—C17—H15	109.5	O6—N3—O5	121.5 (3)
O4—C17—H16	109.5	O7—N3—O5	115.1 (3)
H15—C17—H16	109.5	O6—N3—Er1	178.1 (2)
O4—C17—H17	109.5	O7—N3—Er1	58.24 (15)
H15—C17—H17	109.5	O5—N3—Er1	56.87 (16)
H16—C17—H17	109.5	O9—N4—O8	122.3 (3)
O2—C18—H18	109.5	O9—N4—O10	122.0 (3)
O2—C18—H19	109.5	O8—N4—O10	115.7 (2)
H18—C18—H19	109.5	O9—N4—Er1	177.1 (2)
O2—C18—H20	109.5	O8—N4—Er1	58.09 (13)
H18—C18—H20	109.5	O10—N4—Er1	57.67 (14)
H19—C18—H20	109.5	O12—N5—O13	122.0 (2)
O3—Er1—O1	75.02 (7)	O12—N5—O11	122.1 (2)
O3—Er1—O10	94.30 (7)	O13—N5—O11	115.8 (2)
O1—Er1—O10	146.42 (8)	O12—N5—Er1	179.17 (19)
O3—Er1—O5	75.82 (7)	O13—N5—Er1	58.18 (13)
O1—Er1—O5	72.48 (8)	O11—N5—Er1	57.65 (13)
O10—Er1—O5	136.56 (9)	C1—O1—Er1	126.89 (16)
O3—Er1—O8	141.41 (8)	C2—O2—C18	117.5 (2)
O1—Er1—O8	142.88 (8)	C2—O2—Er1	116.64 (14)
O10—Er1—O8	51.00 (7)	C18—O2—Er1	125.79 (19)
O5—Er1—O8	115.70 (8)	C16—O3—Er1	128.54 (15)
O3—Er1—O11	117.19 (6)	C15—O4—C17	117.2 (2)
O1—Er1—O11	81.46 (8)	C15—O4—Er1	113.57 (14)
O10—Er1—O11	75.35 (8)	C17—O4—Er1	128.36 (18)
O5—Er1—O11	146.82 (8)	N3—O5—Er1	97.71 (18)
O8—Er1—O11	74.41 (9)	N3—O7—Er1	96.36 (16)
O3—Er1—O13	66.82 (6)	N4—O8—Er1	96.54 (16)
O1—Er1—O13	75.74 (8)	N4—O10—Er1	96.69 (17)
O10—Er1—O13	70.83 (8)	N5—O11—Er1	96.68 (14)
O5—Er1—O13	135.84 (7)	N5—O13—Er1	96.42 (15)

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N2—H2 \cdots O3	0.85 (1)	1.89 (3)	2.574 (3)	137 (3)
N1—H1 \cdots O1	0.85 (1)	1.84 (2)	2.567 (3)	143 (3)
C7—H7 \cdots O5 ⁱ	0.93	2.33	3.073 (3)	137.
C9—H9A \cdots O12 ⁱⁱ	0.97	2.50	3.241 (3)	133.

supplementary materials

C10—H10...O9 ⁱⁱⁱ	0.93	2.57	3.395 (4)	148.
C14—H14...O12 ^{iv}	0.93	2.50	3.341 (4)	150.

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

Fig. 1

