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

**Ting Gao, Guang-Ming Li, Po Gao, Peng-Fei Yan* and Guang-Feng Hou**

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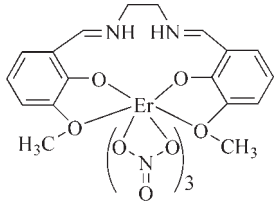
Key indicators: single-crystal X-ray study; $T$ = 291 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.022; $wR$ factor = 0.049; data-to-parameter ratio = 15.6.

In the mononuclear salen-type complex, $[Er(NO_3)_3(C_{18}H_{20}N_2O_4)]$, 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 N—H···O hydrogen bonds occur. The crystal structure is stabilized by intermolecular C—H···O hydrogen bonds.

## Related literature

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




## Experimental

### Crystal data

$[Er(NO_3)_3(C_{18}H_{20}N_2O_4)]$
$M_r$ = 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) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 3.63 mm$^{-1}$
$T$ = 291 K
0.37 × 0.36 × 0.34 mm

### Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min}$ = 0.344, $T_{max}$ = 0.368
21792 measured reflections
5358 independent reflections
4748 reflections with $I > 2\sigma(I)$
$R_{int}$ = 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
$\Delta\rho_{max}$ = 0.97 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.32 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N2—H2···O3 | 0.85 (1) | 1.89 (3) | 2.574 (3) | 137 (3) |
| N1—H1···O1 | 0.85 (1) | 1.84 (2) | 2.567 (3) | 143 (3) |
| C7—H7···O5$^{i}$ | 0.93 | 2.33 | 3.073 (3) | 137 |
| C9—H9$A$···O12$^{ii}$ | 0.97 | 2.50 | 3.241 (3) | 133 |
| 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) $x-\frac{1}{2}, -y+\frac{3}{2}, z+\frac{1}{2}$; (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/MSC, 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).

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# supporting information

*Acta Cryst.* (2010). E**66**, m107 [https://doi.org/10.1107/S1600536809055184]

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

**Ting Gao, Guang-Ming Li, Po Gao, Peng-Fei Yan and Guang-Feng Hou**

### S1. 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···O and C—H···O hydrogen bonds (Table 1).

### S2. 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 for $C_{18}H_{20}Er_1N_5O_{13}$: C 31.72, H 2.96, N 10.27%; found: C 32.08, H 3.00, N 10.38%.

### S3. 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 = 0.97Å (methylene C), and with $U_{iso}$(H) = 1.2Ueq(C) or C—H = 0.96 Å (methyl C) and with $U_{iso}$(H) = 1.5Ueq(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.

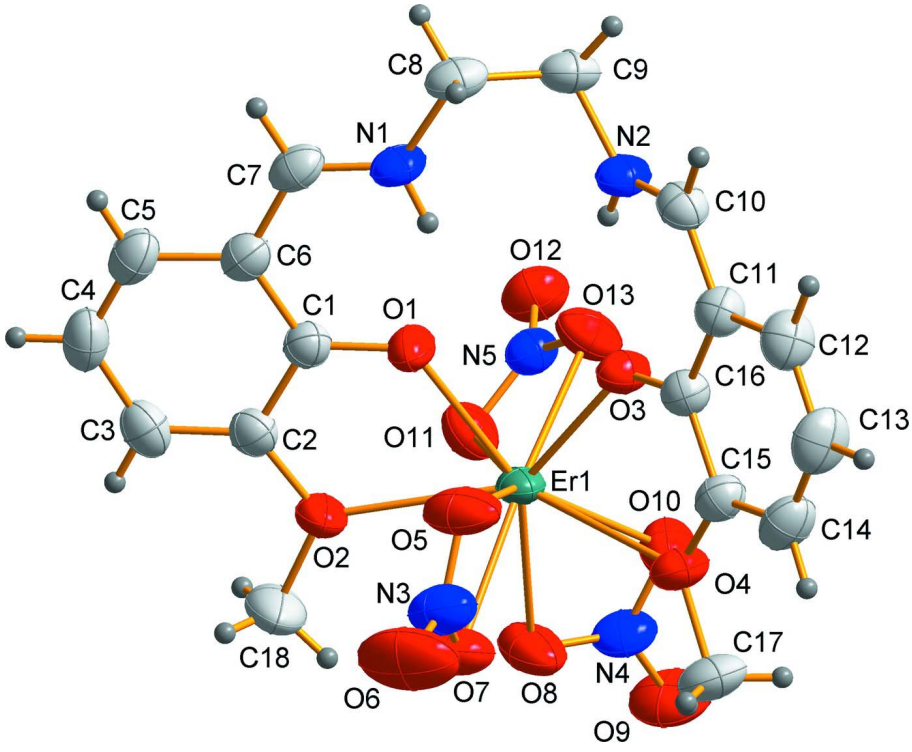


**Figure 1**

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

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

*Crystal data*

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$c = 14.571$ (3) Å
$\beta = 103.98$ (3)°
$V = 2365.1$ (8) Å$^3$
$Z = 4$
$F(000) = 1340$
$D_x = 1.914$ 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 × 0.36 × 0.34 mm

*Data collection*

Rigaku R-AXIS RAPID diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 10.000 pixels mm$^{-1}$
$\omega$ 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 $I > 2\sigma(I)$
$R_{int} = 0.024$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.4°$
$h = -18 \rightarrow 18$
$k = -15 \rightarrow 13$
$l = -18 \rightarrow 18$

*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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| 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) |
| 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 (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| 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, º)*

| | | | |
|---|---|---|---|
| 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) |

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| 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) |
| 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) |

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| 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) |

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| 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) |

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| 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 (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H2···O3 | 0.85 (1) | 1.89 (3) | 2.574 (3) | 137 (3) |
| N1—H1···O1 | 0.85 (1) | 1.84 (2) | 2.567 (3) | 143 (3) |
| C7—H7···O5$^{i}$ | 0.93 | 2.33 | 3.073 (3) | 137 |
| C9—H9*A*···O12$^{ii}$ | 0.97 | 2.50 | 3.241 (3) | 133 |
| 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.