Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# 1,10-Phenanthrolin-1-ium nitrate–aqua-bis(4-hydroxybenzoato-$\kappa^2O,O'$)(nitrato-$\kappa^2O,O'$)(1,10-phenanthroline-$\kappa^2N,N'$)-erbium(III)–1,10-phenanthroline–water (1/1/0.5/2)

**Fwu Ming Shen[a] and Shie Fu Lush[b]***

[a]Department of Biotechnology, Yuanpei University, HsinChu 30015, Taiwan, and [b]Department of Genernal Eduction Center, Yuanpei University, HsinChu 30015, Taiwan
Correspondence e-mail: lush@mail.ypu.edu.tw

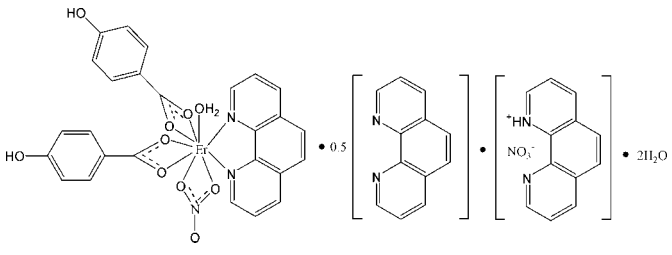
Received 22 November 2010; accepted 10 December 2010

Key indicators: single-crystal X-ray study; $T$ = 97 K; mean $\sigma$(C–C) = 0.010 Å; disorder in main residue; $R$ factor = 0.038; $wR$ factor = 0.105; data-to-parameter ratio = 13.2.

In the title compound, $C_{12}H_9N_2^+\cdot NO_3^-\cdot[Er(C_7H_5O_3)_2(NO_3)(C_{12}H_8N_2)(H_2O)]\cdot0.5C_{12}H_8N_2\cdot2H_2O$, the water-molecule-coordinated $Er^{III}$ ion is chelated by one 1,10-phenanthroline (phen) ligand, two 4-hydroxybenzoate anions and one nitrate anion in a monocapped square-antiprismatic coordination geometry. The uncoordinating phen molecule is approximately parallel to the 1,10-phenanthrolin-1-ium (Hphen) anion [dihedral angle = 3.3 (4)°]. The centroid–centroid distance of 3.801 (5) Å between pyridine rings suggests the existence of $\pi$–$\pi$ stacking. The crystal structure contains an extensive network of classical O—H···O and N—H···O and weak C—H···O hydrogen bonds. C—H···$\pi$ interactions between phen and 4-hydroxybenzoate is also present in the crystal structure. In the crystal, the uncoordinating phen is equally disordered over two sites about an inversion center.

## Related literature

For a related hydrothermal substitution reaction, see: Xiong *et al.* (2001). For related structures, see: Liu *et al.* (2007, 2010); Neelgund *et al.* (2007).



## Experimental

### Crystal data

$C_{12}H_9N_2^+\cdot NO_3^-\cdot[Er(C_7H_5O_3)_2(NO_3)(C_{12}H_8N_2)(H_2O)]\cdot0.5C_{12}H_8N_2\cdot2H_2O$
$M_r$ = 1071.07
Triclinic, $P\overline{1}$
$a$ = 10.9464 (2) Å
$b$ = 11.3682 (3) Å
$c$ = 19.2638 (5) Å
$\alpha$ = 77.108 (2)°
$\beta$ = 84.790 (2)°
$\gamma$ = 67.250 (2)°
$V$ = 2154.95 (10) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 2.03 mm$^{-1}$
$T$ = 97 K
0.35 × 0.20 × 0.18 mm

### Data collection

Oxford Diffraction Gemini-S CCD diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2009)
$T_{min}$ = 0.629, $T_{max}$ = 0.694
16237 measured reflections
7710 independent reflections
6632 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.028

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.105
$S$ = 1.05
7710 reflections
583 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 2.48 e Å$^{-3}$
$\Delta\rho_{min}$ = −1.41 e Å$^{-3}$

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Er1—O1 | 2.470 (4) | Er1—O6 | 2.366 (4) |
| Er1—O2 | 2.376 (4) | Er1—O7 | 2.433 (4) |
| Er1—O3*W* | 2.358 (3) | Er1—N1 | 2.461 (4) |
| Er1—O4 | 2.372 (3) | Er1—N2 | 2.489 (4) |
| Er1—O5 | 2.399 (3) | | |

**Table 2**
Hydrogen-bond geometry (Å, °).

*Cg*4 is the centroid of the C32–C37 ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1*W*—H1*A*···O2$^{i}$ | 0.82 | 2.55 | 3.270 (6) | 148 |
| O1*W*—H1*A*···O6$^{i}$ | 0.82 | 2.22 | 2.875 (6) | 137 |
| O1*W*—H1*B*···O12$^{i}$ | 0.82 | 2.06 | 2.872 (10) | 172 |
| O2*W*—H2*A*···O9$^{ii}$ | 0.82 | 1.94 | 2.737 (8) | 164 |
| O2*W*—H2*B*···O11$^{i}$ | 0.82 | 2.01 | 2.789 (10) | 157 |
| O3*W*—H3*A*···O5$^{iii}$ | 0.82 | 1.90 | 2.671 (5) | 155 |
| O3*W*—H3*B*···O7$^{iii}$ | 0.82 | 2.16 | 2.836 (5) | 140 |
| N4—H4···O2*W* | 0.86 | 1.91 | 2.725 (9) | 157 |
| O8—H8···O1*W*$^{iv}$ | 0.82 | 1.87 | 2.659 (6) | 160 |
| O9—H9···O11$^{v}$ | 0.82 | 2.09 | 2.803 (12) | 145 |
| O9—H9···O12$^{v}$ | 0.82 | 2.43 | 3.172 (12) | 151 |
| C34—H34···O3$^{v}$ | 0.93 | 2.43 | 3.256 (8) | 148 |
| C48—H48···O12$^{vi}$ | 0.93 | 2.27 | 3.046 (11) | 141 |
| C62—H62···O1$^{vii}$ | 0.93 | 2.55 | 3.387 (10) | 150 |
| C70—H70···O13$^{i}$ | 0.93 | 2.35 | 3.244 (13) | 161 |
| C83—H83···*Cg*4$^{ii}$ | 0.93 | 2.78 | 3.628 (9) | 152 |

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $x+1, y, z$; (iii) $-x, -y+1, -z$; (iv) $x-1, y+1, z-1$; (v) $x-1, y, z$; (vi) $x, y-1, z$; (vii) $x, y+1, z$.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2008); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2008); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997);

software used to prepare material for publication: *PLATON* (Spek, 2009).

This work was supported financially by Yuanpei University, Taiwan.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5103).

## References

Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Liu, J.-L., Liu, J.-F. & Zhao, G.-L. (2010). *Acta Cryst.* E**66**, m1513.
Liu, Y.-F., Xia, H.-T., Wang, D.-Q., Yang, S.-P. & Meng, Y.-L. (2007). *Acta Cryst.* E**63**, m2544.
Neelgund, G. M., Shivashankar, S. A., Narasimhamurthy, T. & Rathore, R. S. (2007). *Acta Cryst.* C**63**, m74–m76.
Oxford Diffraction (2008). *CrysAlis CCD* and *CrysAlis RED*. Oxford Diffraction Ltd, Yarnton, England.
Oxford Diffraction (2009). *CrysAlis PRO*. Oxford Diffraction Ltd, Yarnton, England.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Xiong, R.-G., Zhang, J., Chen, Z.-F., You, X.-Z., Che, C.-M. & Fun, H. K. (2001). *J. Chem. Soc. Dalton Trans.* pp. 780–782.

# supplementary materials

*Acta Cryst.* (2011). E**67**, m86-m87 [ **doi:10.1107/S1600536810051767** ]

# 1,10-Phenanthrolin-1-ium nitrate-aquabis(4-hydroxybenzoato-$\kappa^2O,O'$)(nitrato-$\kappa^2O,O'$)(1,10-phenanthroline-$\kappa^2N,N'$)erbium(III)-1,10-phenanthroline-water (1/1/0.5/2)

**F. M. Shen and S. F. Lush**

## Comment

The coordination chemistry of erbium (III) with N and O donor ligands has been investigated in the past decade and numbers of erbium (III) complexes with different donor ligands have been synthesized and studied by X-ray crystallography (Liu *et al.*, 2010; Neelgund *et al.*, 2007; Liu *et al.*, 2007). The title compound was recently obtained from the reaction of erbium nitrate, sodium benzoate and phen in an methanol-water mixture, and its crystal structure is reported here. Since no 4-hydrobenzoic acid ligand is present in the starting reaction mixture, it may be derived from the benzoic acid *via in situ* substitution(Xiong *et al.*, 2001) under hydrothermal condition.

The $Er^{III}$ ion is nine-coordinated by two N atoms of a phen ligand, four carboxylate O atoms of two 4-hydroxybenzoate anions, two O atoms of nitrate anion and one O atom of a water molecule. The resulting coordination geometry is a monocapped square antiprismatic coordination (Table 1 and Fig. 1).

The phen molecule is approximately parallel to 1,10-phenanthrolinium (Hphen), making dihedral angle of 3.3 (4)°.The centroid-centroid distance between N4-pyridine and N7-pyridine rings is 3.801 (5) Å, indictative of π—π interaction.The crystal structure contain an extensive network of classical (O—H···O, N—H···O) and weak (C—H···O) hydrogen bonds (Table 2 and Fig. 2).

In addition, C—H···π interaction (C83—H83···*Cg*4(C32—C37); full details and symmetry code are given in Table 2.) between phen and 4-hydroxybenzoate is present in the crystal structure.

## Experimental

Erbium trinitrate solution was prepared by dissolving $Er(NO_3)_3.6H_2O$ (0.4631 g, 1.00 mmole) at room temperature with stirring. The ligand solution was prepared by dissolving benzoic acid (0.4889 g, 4 mmole) and 1,10-phenanthroline (4 mmole) in 20 ml methanol at room temperature. The pH of the ligand solution was adjusted to about 6 with 2 N NaOH. The Er solution was added drop wise and slowly to the ligand solution. The reaction mixture was stirred for 2 h at room temperature. Pink crystals were obtained at room temperature over a period 3 months.

## Refinement

Position C82, N6, C86, N7, C87 and C88 of the phen ring split into two different atoms with 50% occupancies for each, respectively. H atoms bonded to O and N atoms were placed in calculated positions and refined with the distances constrains of O—H = 0.82, N—H = 0.86 Å, and $U_{iso}$(H)= 1.2$U_{eq}$(N) and 1.5$U_{eq}$(O). Other H atoms were positioned geometrically with C—H = 0.93 Å and refined using a riding model with $U_{iso}$(H) = 1.2$U_{eq}$(C).

**Figures**

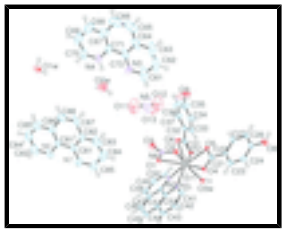


Fig. 1. View of the title compound with the atom numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level [symmetry code: (i) 2 - *x*, -*y*, 1 - *z*].

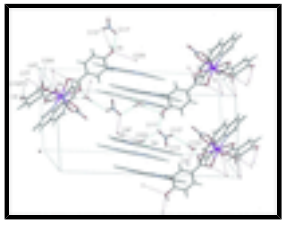


Fig. 2. The molecular packing for the title compound. Hydrogen bonds are shown as dashed lines.

## 1,10-Phenanthrolin-1-ium nitrate– aquabis(4-hydroxybenzoato-$\kappa^2O,O'$)(nitrato- $\kappa^2O,O'$)(1,10-phenanthroline-$\kappa^2N,N'$)erbium(III)–\1,10-phenanthroline–water (1/1/0.5/2)

*Crystal data*

| | |
|---|---|
| $C_{12}H_9N_2^+\cdot NO_3^-\cdot[Er(C_7H_5O_3)_2(NO_3)(C_{12}H_8N_2)(H_2O)]\cdot 0.5C_{12}H_8N_2\cdot 2H_2O$ | $Z = 2$ |
| $M_r = 1071.07$ | $F(000) = 1076$ |
| Triclinic, $P\overline{1}$ | $D_x = 1.651$ Mg m$^{-3}$ |
| Hall symbol: -P 1 | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| $a = 10.9464$ (2) Å | Cell parameters from 12670 reflections |
| $b = 11.3682$ (3) Å | $\theta = 2.4$–$29.2°$ |
| $c = 19.2638$ (5) Å | $\mu = 2.03$ mm$^{-1}$ |
| $\alpha = 77.108$ (2)° | $T = 97$ K |
| $\beta = 84.790$ (2)° | Block, pink |
| $\gamma = 67.250$ (2)° | 0.35 × 0.20 × 0.18 mm |
| $V = 2154.95$ (10) Å$^3$ | |

*Data collection*

| | |
|---|---|
| Oxford Diffraction Gemini-S CCD diffractometer | 7710 independent reflections |
| Radiation source: fine-focus sealed tube | 6632 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.028$ |
| Detector resolution: 9 pixels mm$^{-1}$ | $\theta_{max} = 25.2°$, $\theta_{min} = 2.5°$ |
| ω scans | $h = -13\rightarrow13$ |
| Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2009) | $k = -13\rightarrow11$ |
| $T_{min} = 0.629$, $T_{max} = 0.694$ | $l = -23\rightarrow22$ |
| 16237 measured reflections | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.038$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.105$ | H-atom parameters constrained |
| $S = 1.05$ | $w = 1/[\sigma^2(F_o^2) + (0.0656P)^2 + 2.9468P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 7710 reflections | $(\Delta/\sigma)_{max} = 0.001$ |
| 583 parameters | $\Delta\rho_{max} = 2.48$ e Å$^{-3}$ |
| 0 restraints | $\Delta\rho_{min} = -1.41$ e Å$^{-3}$ |

*Special details*

**Geometry**. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

**Refinement**. Refinement on $F^2$ for ALL reflections except those flagged by the user for potential systematic errors. Weighted *R*-factors *wR* and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating -*R*-factor-obs *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* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| Er1 | 0.23247 (2) | 0.40305 (2) | 0.07892 (1) | 0.0145 (1) | |
| O1 | 0.3934 (4) | 0.3029 (4) | 0.17753 (19) | 0.0232 (11) | |
| O2 | 0.3711 (3) | 0.4927 (4) | 0.11782 (19) | 0.0234 (11) | |
| O3 | 0.4913 (4) | 0.4118 (5) | 0.2139 (2) | 0.0406 (16) | |
| O3W | 0.1453 (3) | 0.3643 (3) | −0.01739 (18) | 0.0176 (10) | |
| O4 | 0.2763 (3) | 0.5363 (3) | −0.02595 (18) | 0.0199 (11) | |
| O5 | 0.0975 (3) | 0.6273 (3) | 0.03472 (18) | 0.0176 (11) | |
| O6 | 0.1303 (3) | 0.4721 (4) | 0.18419 (18) | 0.0204 (11) | |
| O7 | 0.0106 (3) | 0.4202 (3) | 0.12003 (18) | 0.0178 (11) | |
| O8 | 0.0969 (4) | 1.1108 (4) | −0.2073 (2) | 0.0379 (14) | |
| O9 | −0.4015 (6) | 0.6324 (7) | 0.3624 (3) | 0.084 (3) | |
| N1 | 0.4400 (4) | 0.2592 (4) | 0.0322 (2) | 0.0166 (12) | |
| N2 | 0.2730 (4) | 0.1678 (4) | 0.1217 (2) | 0.0200 (12) | |
| N8 | 0.4204 (4) | 0.4033 (5) | 0.1714 (2) | 0.0224 (16) | |
| C21 | 0.1771 (5) | 0.6361 (5) | −0.0180 (3) | 0.0165 (16) | |
| C22 | 0.1524 (5) | 0.7613 (5) | −0.0678 (3) | 0.0165 (16) | |
| C23 | 0.2377 (5) | 0.7697 (5) | −0.1251 (3) | 0.0209 (17) | |
| C24 | 0.2173 (6) | 0.8873 (6) | −0.1703 (3) | 0.0265 (17) | |

| | | | | | |
|---|---|---|---|---|---|
| C25 | 0.1121 (5) | 0.9991 (5) | −0.1603 (3) | 0.0240 (17) | |
| C26 | 0.0270 (5) | 0.9913 (5) | −0.1026 (3) | 0.0204 (17) | |
| C27 | 0.0462 (5) | 0.8744 (5) | −0.0570 (3) | 0.0189 (16) | |
| C31 | 0.0201 (5) | 0.4661 (5) | 0.1733 (3) | 0.0173 (17) | |
| C32 | −0.0930 (5) | 0.5123 (5) | 0.2214 (3) | 0.0188 (17) | |
| C33 | −0.2127 (5) | 0.5001 (5) | 0.2132 (3) | 0.0233 (17) | |
| C34 | −0.3172 (6) | 0.5408 (6) | 0.2595 (3) | 0.0302 (19) | |
| C35 | −0.3038 (7) | 0.5950 (8) | 0.3140 (4) | 0.048 (3) | |
| C36 | −0.1851 (7) | 0.6091 (8) | 0.3221 (4) | 0.048 (3) | |
| C37 | −0.0815 (6) | 0.5674 (6) | 0.2763 (3) | 0.0307 (19) | |
| C41 | 0.5172 (5) | 0.3009 (5) | −0.0162 (3) | 0.0196 (16) | |
| C42 | 0.6408 (5) | 0.2174 (6) | −0.0376 (3) | 0.0232 (16) | |
| C43 | 0.6854 (5) | 0.0893 (5) | −0.0062 (3) | 0.0234 (16) | |
| C44 | 0.6101 (5) | 0.0409 (5) | 0.0460 (3) | 0.0226 (17) | |
| C45 | 0.6523 (6) | −0.0923 (6) | 0.0828 (3) | 0.0282 (17) | |
| C46 | 0.5745 (6) | −0.1344 (6) | 0.1304 (3) | 0.0323 (19) | |
| C47 | 0.4424 (6) | −0.0499 (5) | 0.1450 (3) | 0.0247 (17) | |
| C48 | 0.3541 (6) | −0.0925 (6) | 0.1906 (3) | 0.0315 (19) | |
| C49 | 0.2285 (6) | −0.0087 (6) | 0.1985 (3) | 0.0282 (17) | |
| C50 | 0.1909 (5) | 0.1214 (6) | 0.1633 (3) | 0.0241 (17) | |
| C51 | 0.3980 (5) | 0.0820 (5) | 0.1119 (3) | 0.0186 (17) | |
| C52 | 0.4844 (5) | 0.1306 (5) | 0.0621 (3) | 0.0176 (16) | |
| N6 | 0.9403 (6) | 0.1675 (6) | 0.4488 (3) | 0.0379 (19) | 0.500 |
| N7 | 0.9737 (6) | −0.0343 (6) | 0.4147 (3) | 0.0373 (19) | 0.500 |
| C81 | 0.9773 (6) | 0.0350 (6) | 0.4644 (3) | 0.0307 (17) | |
| C82 | 0.9403 (6) | 0.1675 (6) | 0.4488 (3) | 0.0379 (19) | 0.500 |
| C83 | 0.8975 (7) | 0.2307 (8) | 0.3798 (4) | 0.050 (3) | |
| C84 | 0.8912 (8) | 0.1665 (9) | 0.3303 (4) | 0.054 (3) | |
| C85 | 0.9291 (7) | 0.0356 (9) | 0.3474 (4) | 0.050 (3) | |
| C86 | 0.9737 (6) | −0.0343 (6) | 0.4147 (3) | 0.0373 (19) | 0.500 |
| C87 | 0.9379 (12) | 0.2441 (15) | 0.5036 (8) | 0.049 (5) | 0.500 |
| C88 | 0.9813 (13) | 0.1792 (15) | 0.5675 (8) | 0.045 (5) | 0.500 |
| N3 | 0.6566 (5) | 0.8871 (7) | 0.4088 (3) | 0.047 (2) | |
| N4 | 0.7372 (5) | 0.7810 (6) | 0.5468 (3) | 0.0404 (19) | |
| C61 | 0.6104 (7) | 0.9421 (10) | 0.3441 (4) | 0.075 (2) | |
| C62 | 0.5602 (7) | 1.0749 (10) | 0.3179 (5) | 0.075 (2) | |
| C63 | 0.5605 (7) | 1.1543 (11) | 0.3588 (5) | 0.075 (2) | |
| C64 | 0.6096 (6) | 1.1019 (8) | 0.4282 (4) | 0.053 (3) | |
| C65 | 0.6144 (8) | 1.1804 (9) | 0.4766 (6) | 0.075 (4) | |
| C66 | 0.6588 (9) | 1.1252 (10) | 0.5436 (6) | 0.072 (4) | |
| C67 | 0.7030 (7) | 0.9884 (9) | 0.5694 (4) | 0.049 (3) | |
| C68 | 0.7458 (8) | 0.9284 (12) | 0.6377 (4) | 0.069 (4) | |
| C69 | 0.7839 (8) | 0.7975 (12) | 0.6597 (4) | 0.072 (4) | |
| C70 | 0.7774 (7) | 0.7261 (9) | 0.6133 (4) | 0.056 (3) | |
| C71 | 0.7003 (5) | 0.9088 (7) | 0.5234 (3) | 0.0334 (19) | |
| C72 | 0.6538 (6) | 0.9681 (7) | 0.4511 (3) | 0.041 (2) | |
| O11 | 0.4009 (8) | 0.5285 (9) | 0.3933 (4) | 0.1090 (19) | |
| O12 | 0.3154 (8) | 0.6897 (9) | 0.3035 (4) | 0.1090 (19) | |
| O13 | 0.2058 (8) | 0.5725 (9) | 0.3489 (4) | 0.1090 (19) | |

| | | | | | |
|---|---|---|---|---|---|
| N5 | 0.3076 (11) | 0.6002 (11) | 0.3496 (6) | 0.1090 (19) | |
| O1W | 0.8550 (4) | 0.2838 (4) | 0.8087 (2) | 0.0373 (14) | |
| O2W | 0.7115 (6) | 0.5915 (6) | 0.4911 (3) | 0.070 (2) | |
| H3A | 0.07580 | 0.35180 | −0.01090 | 0.0260* | |
| H3B | 0.13890 | 0.42290 | −0.05230 | 0.0260* | |
| H8 | 0.03190 | 1.17010 | −0.19610 | 0.0560* | |
| H9 | −0.46530 | 0.61790 | 0.35310 | 0.1260* | |
| H23 | 0.30870 | 0.69550 | −0.13270 | 0.0250* | |
| H24 | 0.27510 | 0.89200 | −0.20830 | 0.0320* | |
| H26 | −0.04340 | 1.06600 | −0.09500 | 0.0240* | |
| H27 | −0.01140 | 0.87000 | −0.01880 | 0.0220* | |
| H33 | −0.22230 | 0.46410 | 0.17610 | 0.0280* | |
| H34 | −0.39630 | 0.53160 | 0.25390 | 0.0360* | |
| H36 | −0.17620 | 0.64680 | 0.35860 | 0.0580* | |
| H37 | −0.00240 | 0.57640 | 0.28220 | 0.0370* | |
| H41 | 0.48810 | 0.38930 | −0.03680 | 0.0240* | |
| H42 | 0.69090 | 0.24950 | −0.07260 | 0.0280* | |
| H43 | 0.76710 | 0.03300 | −0.01960 | 0.0280* | |
| H45 | 0.73580 | −0.15070 | 0.07320 | 0.0340* | |
| H46 | 0.60650 | −0.22060 | 0.15490 | 0.0390* | |
| H48 | 0.38160 | −0.17850 | 0.21540 | 0.0380* | |
| H49 | 0.16820 | −0.03750 | 0.22700 | 0.0340* | |
| H50 | 0.10450 | 0.17830 | 0.16920 | 0.0290* | |
| H83 | 0.87210 | 0.32070 | 0.36750 | 0.0600* | |
| H84 | 0.86100 | 0.21180 | 0.28470 | 0.0650* | |
| H85 | 0.92510 | −0.00870 | 0.31300 | 0.0590* | |
| H87 | 0.90650 | 0.33460 | 0.49240 | 0.0580* | 0.500 |
| H88 | 0.98420 | 0.22370 | 0.60200 | 0.0540* | 0.500 |
| H4 | 0.73500 | 0.73310 | 0.51850 | 0.0480* | |
| H61 | 0.61150 | 0.88810 | 0.31400 | 0.0890* | |
| H62 | 0.52650 | 1.10840 | 0.27200 | 0.0890* | |
| H63 | 0.52850 | 1.24390 | 0.34160 | 0.0890* | |
| H65 | 0.58650 | 1.27020 | 0.46130 | 0.0890* | |
| H66 | 0.66070 | 1.17790 | 0.57380 | 0.0860* | |
| H68 | 0.74870 | 0.97820 | 0.66940 | 0.0820* | |
| H69 | 0.81410 | 0.75720 | 0.70580 | 0.0860* | |
| H70 | 0.80180 | 0.63660 | 0.62860 | 0.0670* | |
| H1A | 0.82320 | 0.35200 | 0.82330 | 0.0560* | |
| H1B | 0.80360 | 0.28640 | 0.77950 | 0.0560* | |
| H2A | 0.68500 | 0.58770 | 0.45350 | 0.1050* | |
| H2B | 0.69560 | 0.53770 | 0.52280 | 0.1050* | |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Er1 | 0.0110 (1) | 0.0126 (1) | 0.0177 (1) | −0.0017 (1) | −0.0013 (1) | −0.0031 (1) |
| O1 | 0.0243 (19) | 0.018 (2) | 0.026 (2) | −0.0047 (16) | −0.0082 (16) | −0.0046 (16) |
| O2 | 0.0178 (18) | 0.026 (2) | 0.023 (2) | −0.0060 (16) | −0.0008 (15) | −0.0020 (16) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O3 | 0.039 (2) | 0.045 (3) | 0.045 (3) | −0.017 (2) | −0.019 (2) | −0.014 (2) |
| O3W | 0.0143 (17) | 0.0174 (19) | 0.0191 (18) | −0.0043 (15) | −0.0005 (14) | −0.0025 (15) |
| O4 | 0.0135 (17) | 0.0150 (19) | 0.025 (2) | 0.0005 (15) | 0.0031 (14) | −0.0037 (15) |
| O5 | 0.0125 (17) | 0.0163 (19) | 0.0219 (19) | −0.0042 (14) | 0.0000 (14) | −0.0022 (15) |
| O6 | 0.0158 (18) | 0.024 (2) | 0.0207 (19) | −0.0077 (16) | −0.0009 (14) | −0.0024 (15) |
| O7 | 0.0178 (18) | 0.0184 (19) | 0.0170 (18) | −0.0071 (15) | 0.0021 (14) | −0.0039 (15) |
| O8 | 0.047 (3) | 0.019 (2) | 0.035 (2) | −0.0078 (19) | 0.015 (2) | 0.0048 (18) |
| O9 | 0.058 (4) | 0.148 (7) | 0.097 (5) | −0.067 (4) | 0.056 (3) | −0.096 (5) |
| N1 | 0.012 (2) | 0.016 (2) | 0.022 (2) | −0.0026 (17) | −0.0039 (17) | −0.0077 (18) |
| N2 | 0.019 (2) | 0.019 (2) | 0.023 (2) | −0.0070 (19) | −0.0034 (18) | −0.0052 (19) |
| N8 | 0.012 (2) | 0.028 (3) | 0.028 (3) | −0.004 (2) | −0.0001 (19) | −0.014 (2) |
| C21 | 0.014 (2) | 0.017 (3) | 0.018 (3) | −0.004 (2) | −0.003 (2) | −0.005 (2) |
| C22 | 0.013 (2) | 0.014 (3) | 0.023 (3) | −0.005 (2) | −0.003 (2) | −0.004 (2) |
| C23 | 0.019 (3) | 0.020 (3) | 0.022 (3) | −0.006 (2) | 0.001 (2) | −0.004 (2) |
| C24 | 0.030 (3) | 0.028 (3) | 0.022 (3) | −0.013 (3) | 0.011 (2) | −0.007 (2) |
| C25 | 0.028 (3) | 0.019 (3) | 0.024 (3) | −0.010 (2) | −0.001 (2) | 0.000 (2) |
| C26 | 0.019 (3) | 0.012 (3) | 0.027 (3) | −0.001 (2) | −0.001 (2) | −0.006 (2) |
| C27 | 0.014 (2) | 0.020 (3) | 0.021 (3) | −0.005 (2) | 0.004 (2) | −0.005 (2) |
| C31 | 0.021 (3) | 0.012 (3) | 0.017 (3) | −0.006 (2) | −0.002 (2) | 0.001 (2) |
| C32 | 0.019 (3) | 0.015 (3) | 0.020 (3) | −0.006 (2) | 0.001 (2) | 0.000 (2) |
| C33 | 0.027 (3) | 0.014 (3) | 0.027 (3) | −0.007 (2) | 0.001 (2) | −0.002 (2) |
| C34 | 0.023 (3) | 0.034 (3) | 0.040 (4) | −0.017 (3) | 0.010 (3) | −0.013 (3) |
| C35 | 0.041 (4) | 0.068 (5) | 0.055 (4) | −0.035 (4) | 0.027 (3) | −0.038 (4) |
| C36 | 0.049 (4) | 0.078 (6) | 0.044 (4) | −0.042 (4) | 0.023 (3) | −0.041 (4) |
| C37 | 0.030 (3) | 0.041 (4) | 0.029 (3) | −0.020 (3) | 0.008 (2) | −0.014 (3) |
| C41 | 0.016 (2) | 0.020 (3) | 0.025 (3) | −0.007 (2) | −0.002 (2) | −0.008 (2) |
| C42 | 0.013 (2) | 0.027 (3) | 0.033 (3) | −0.008 (2) | 0.003 (2) | −0.013 (2) |
| C43 | 0.013 (2) | 0.023 (3) | 0.036 (3) | −0.001 (2) | −0.001 (2) | −0.020 (3) |
| C44 | 0.015 (3) | 0.018 (3) | 0.035 (3) | 0.000 (2) | −0.009 (2) | −0.014 (2) |
| C45 | 0.023 (3) | 0.018 (3) | 0.039 (3) | 0.002 (2) | −0.009 (3) | −0.011 (3) |
| C46 | 0.037 (3) | 0.014 (3) | 0.039 (4) | 0.001 (3) | −0.013 (3) | −0.006 (3) |
| C47 | 0.033 (3) | 0.015 (3) | 0.025 (3) | −0.007 (2) | −0.010 (2) | −0.002 (2) |
| C48 | 0.049 (4) | 0.018 (3) | 0.028 (3) | −0.014 (3) | −0.013 (3) | 0.002 (2) |
| C49 | 0.038 (3) | 0.025 (3) | 0.026 (3) | −0.017 (3) | −0.002 (2) | −0.004 (2) |
| C50 | 0.025 (3) | 0.028 (3) | 0.022 (3) | −0.012 (2) | −0.002 (2) | −0.006 (2) |
| C51 | 0.020 (3) | 0.017 (3) | 0.019 (3) | −0.005 (2) | −0.007 (2) | −0.005 (2) |
| C52 | 0.015 (2) | 0.017 (3) | 0.023 (3) | −0.005 (2) | −0.006 (2) | −0.008 (2) |
| N6 | 0.031 (3) | 0.033 (3) | 0.045 (4) | −0.013 (3) | 0.004 (3) | 0.001 (3) |
| N7 | 0.031 (3) | 0.047 (4) | 0.036 (3) | −0.019 (3) | 0.005 (2) | −0.007 (3) |
| C81 | 0.026 (3) | 0.034 (3) | 0.030 (3) | −0.013 (3) | 0.006 (2) | −0.002 (3) |
| C82 | 0.031 (3) | 0.033 (3) | 0.045 (4) | −0.013 (3) | 0.004 (3) | 0.001 (3) |
| C83 | 0.048 (4) | 0.040 (4) | 0.056 (5) | −0.022 (4) | 0.001 (4) | 0.014 (4) |
| C84 | 0.055 (5) | 0.068 (6) | 0.037 (4) | −0.033 (4) | −0.011 (3) | 0.016 (4) |
| C85 | 0.038 (4) | 0.080 (6) | 0.037 (4) | −0.032 (4) | 0.004 (3) | −0.008 (4) |
| C86 | 0.031 (3) | 0.047 (4) | 0.036 (3) | −0.019 (3) | 0.005 (2) | −0.007 (3) |
| C87 | 0.022 (6) | 0.047 (9) | 0.054 (9) | −0.005 (6) | −0.003 (6) | 0.022 (7) |
| C88 | 0.032 (7) | 0.049 (9) | 0.053 (9) | −0.016 (7) | 0.006 (6) | −0.011 (7) |
| N3 | 0.036 (3) | 0.070 (5) | 0.027 (3) | −0.016 (3) | 0.000 (2) | 0.001 (3) |
| N4 | 0.029 (3) | 0.050 (4) | 0.030 (3) | −0.008 (3) | 0.000 (2) | 0.003 (3) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C61 | 0.029 (2) | 0.106 (5) | 0.052 (3) | −0.012 (3) | 0.003 (2) | 0.030 (3) |
| C62 | 0.029 (2) | 0.106 (5) | 0.052 (3) | −0.012 (3) | 0.003 (2) | 0.030 (3) |
| C63 | 0.029 (2) | 0.106 (5) | 0.052 (3) | −0.012 (3) | 0.003 (2) | 0.030 (3) |
| C64 | 0.022 (3) | 0.043 (5) | 0.066 (5) | −0.001 (3) | 0.013 (3) | 0.016 (4) |
| C65 | 0.046 (5) | 0.043 (5) | 0.120 (9) | −0.013 (4) | 0.040 (5) | −0.010 (6) |
| C66 | 0.056 (5) | 0.061 (6) | 0.112 (8) | −0.032 (5) | 0.043 (6) | −0.044 (6) |
| C67 | 0.028 (3) | 0.071 (6) | 0.054 (5) | −0.020 (4) | 0.013 (3) | −0.026 (4) |
| C68 | 0.040 (4) | 0.126 (10) | 0.045 (5) | −0.027 (5) | 0.005 (4) | −0.038 (6) |
| C69 | 0.038 (4) | 0.126 (10) | 0.028 (4) | −0.013 (5) | −0.002 (3) | −0.001 (5) |
| C70 | 0.033 (4) | 0.077 (6) | 0.031 (4) | −0.003 (4) | −0.004 (3) | 0.008 (4) |
| C71 | 0.018 (3) | 0.045 (4) | 0.031 (3) | −0.009 (3) | 0.005 (2) | −0.003 (3) |
| C72 | 0.019 (3) | 0.056 (5) | 0.034 (4) | −0.009 (3) | 0.008 (3) | 0.006 (3) |
| O11 | 0.108 (3) | 0.127 (4) | 0.101 (3) | −0.076 (3) | −0.014 (2) | 0.022 (3) |
| O12 | 0.108 (3) | 0.127 (4) | 0.101 (3) | −0.076 (3) | −0.014 (2) | 0.022 (3) |
| O13 | 0.108 (3) | 0.127 (4) | 0.101 (3) | −0.076 (3) | −0.014 (2) | 0.022 (3) |
| N5 | 0.108 (3) | 0.127 (4) | 0.101 (3) | −0.076 (3) | −0.014 (2) | 0.022 (3) |
| O1W | 0.042 (2) | 0.019 (2) | 0.050 (3) | −0.0106 (19) | 0.003 (2) | −0.0084 (19) |
| O2W | 0.090 (4) | 0.067 (4) | 0.049 (3) | −0.026 (4) | 0.014 (3) | −0.016 (3) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Er1—O1 | 2.470 (4) | C44—C52 | 1.417 (8) |
| Er1—O2 | 2.376 (4) | C44—C45 | 1.431 (8) |
| Er1—O3W | 2.358 (3) | C45—C46 | 1.331 (9) |
| Er1—O4 | 2.372 (3) | C46—C47 | 1.437 (9) |
| Er1—O5 | 2.399 (3) | C47—C51 | 1.399 (8) |
| Er1—O6 | 2.366 (4) | C47—C48 | 1.399 (9) |
| Er1—O7 | 2.433 (4) | C48—C49 | 1.355 (10) |
| Er1—N1 | 2.461 (4) | C49—C50 | 1.396 (9) |
| Er1—N2 | 2.489 (4) | C51—C52 | 1.457 (8) |
| O1—N8 | 1.264 (7) | C23—H23 | 0.9300 |
| O2—N8 | 1.264 (6) | C24—H24 | 0.9300 |
| O3—N8 | 1.221 (6) | C26—H26 | 0.9300 |
| O4—C21 | 1.259 (6) | C27—H27 | 0.9300 |
| O5—C21 | 1.289 (7) | C33—H33 | 0.9300 |
| O6—C31 | 1.273 (7) | C34—H34 | 0.9300 |
| O7—C31 | 1.279 (7) | C36—H36 | 0.9300 |
| O8—C25 | 1.346 (7) | C37—H37 | 0.9300 |
| O9—C35 | 1.356 (10) | C41—H41 | 0.9300 |
| O3W—H3B | 0.8200 | C42—H42 | 0.9300 |
| O3W—H3A | 0.8200 | C43—H43 | 0.9300 |
| O8—H8 | 0.8200 | C45—H45 | 0.9300 |
| O9—H9 | 0.8200 | C46—H46 | 0.9300 |
| O11—N5 | 1.274 (15) | C48—H48 | 0.9300 |
| O12—N5 | 1.217 (14) | C49—H49 | 0.9300 |
| O13—N5 | 1.272 (16) | C50—H50 | 0.9300 |
| O1W—H1A | 0.8200 | C81—C82 | 1.368 (9) |
| O1W—H1B | 0.8200 | C81—C81$^{i}$ | 1.447 (8) |
| N1—C41 | 1.333 (7) | C81—C86 | 1.381 (9) |

| | | | |
|---|---|---|---|
| N1—C52 | 1.353 (7) | C82—C83 | 1.389 (10) |
| N2—C51 | 1.365 (7) | C82—C87 | 1.504 (17) |
| N2—C50 | 1.332 (7) | C83—C84 | 1.345 (12) |
| O2W—H2B | 0.8200 | C84—C85 | 1.350 (13) |
| O2W—H2A | 0.8200 | C85—C86 | 1.381 (10) |
| N6—C81 | 1.368 (9) | C87—C88 | 1.31 (2) |
| N6—C87 | 1.504 (17) | C83—H83 | 0.9300 |
| N6—C83 | 1.389 (10) | C84—H84 | 0.9300 |
| N7—C85 | 1.381 (10) | C85—H85 | 0.9300 |
| N7—C81 | 1.381 (9) | C87—H87 | 0.9300 |
| N3—C61 | 1.312 (10) | C88—H88 | 0.9300 |
| N3—C72 | 1.350 (10) | C61—C62 | 1.380 (15) |
| N4—C71 | 1.328 (10) | C62—C63 | 1.325 (15) |
| N4—C70 | 1.326 (10) | C63—C64 | 1.400 (12) |
| N4—H4 | 0.8600 | C64—C72 | 1.383 (11) |
| C21—C22 | 1.470 (8) | C64—C65 | 1.444 (13) |
| C22—C27 | 1.403 (8) | C65—C66 | 1.346 (16) |
| C22—C23 | 1.391 (8) | C66—C67 | 1.420 (14) |
| C23—C24 | 1.371 (8) | C67—C68 | 1.371 (11) |
| C24—C25 | 1.384 (9) | C67—C71 | 1.410 (11) |
| C25—C26 | 1.394 (8) | C68—C69 | 1.356 (17) |
| C26—C27 | 1.371 (8) | C69—C70 | 1.358 (14) |
| C31—C32 | 1.474 (8) | C71—C72 | 1.448 (8) |
| C32—C37 | 1.381 (8) | C61—H61 | 0.9300 |
| C32—C33 | 1.396 (8) | C62—H62 | 0.9300 |
| C33—C34 | 1.381 (9) | C63—H63 | 0.9300 |
| C34—C35 | 1.375 (10) | C65—H65 | 0.9300 |
| C35—C36 | 1.396 (12) | C66—H66 | 0.9300 |
| C36—C37 | 1.371 (10) | C68—H68 | 0.9300 |
| C41—C42 | 1.408 (8) | C69—H69 | 0.9300 |
| C42—C43 | 1.355 (8) | C70—H70 | 0.9300 |
| C43—C44 | 1.395 (8) | | |
| O1—Er1—O2 | 52.34 (14) | N1—C41—C42 | 123.0 (5) |
| O1—Er1—O3W | 144.85 (13) | C41—C42—C43 | 118.6 (5) |
| O1—Er1—O4 | 120.59 (13) | C42—C43—C44 | 120.7 (5) |
| O1—Er1—O5 | 130.28 (13) | C43—C44—C45 | 123.8 (5) |
| O1—Er1—O6 | 70.36 (13) | C43—C44—C52 | 116.9 (5) |
| O1—Er1—O7 | 111.53 (13) | C45—C44—C52 | 119.3 (5) |
| O1—Er1—N1 | 72.55 (13) | C44—C45—C46 | 121.4 (6) |
| O1—Er1—N2 | 68.63 (14) | C45—C46—C47 | 121.7 (6) |
| O1—Er1—C21 | 129.79 (16) | C46—C47—C51 | 119.0 (6) |
| O1—Er1—C31 | 91.78 (15) | C48—C47—C51 | 117.6 (6) |
| O2—Er1—O3W | 147.75 (12) | C46—C47—C48 | 123.5 (5) |
| O2—Er1—O4 | 75.78 (12) | C47—C48—C49 | 120.1 (6) |
| O2—Er1—O5 | 83.49 (13) | C48—C49—C50 | 119.1 (6) |
| O2—Er1—O6 | 75.18 (13) | N2—C50—C49 | 123.0 (6) |
| O2—Er1—O7 | 128.27 (12) | N2—C51—C47 | 122.5 (5) |
| O2—Er1—N1 | 84.17 (14) | N2—C51—C52 | 117.6 (5) |
| O2—Er1—N2 | 119.87 (14) | C47—C51—C52 | 119.8 (5) |

| | | | |
|---|---|---|---|
| O2—Er1—C21 | 77.53 (15) | C44—C52—C51 | 118.7 (5) |
| O2—Er1—C31 | 101.38 (15) | N1—C52—C51 | 118.5 (5) |
| O3W—Er1—O4 | 72.86 (12) | N1—C52—C44 | 122.8 (5) |
| O3W—Er1—O5 | 84.64 (11) | C22—C23—H23 | 120.00 |
| O3W—Er1—O6 | 130.89 (12) | C24—C23—H23 | 120.00 |
| O3W—Er1—O7 | 77.04 (12) | C25—C24—H24 | 119.00 |
| O3W—Er1—N1 | 81.08 (13) | C23—C24—H24 | 119.00 |
| O3W—Er1—N2 | 80.02 (12) | C25—C26—H26 | 120.00 |
| O3W—Er1—C21 | 78.02 (14) | C27—C26—H26 | 120.00 |
| O3W—Er1—C31 | 103.94 (15) | C22—C27—H27 | 120.00 |
| O4—Er1—O5 | 54.83 (12) | C26—C27—H27 | 120.00 |
| O4—Er1—O6 | 126.38 (13) | C34—C33—H33 | 120.00 |
| O4—Er1—O7 | 123.64 (12) | C32—C33—H33 | 120.00 |
| O4—Er1—N1 | 75.77 (12) | C33—C34—H34 | 120.00 |
| O4—Er1—N2 | 136.77 (12) | C35—C34—H34 | 120.00 |
| O4—Er1—C21 | 27.04 (14) | C35—C36—H36 | 120.00 |
| O4—Er1—C31 | 128.77 (14) | C37—C36—H36 | 120.00 |
| O5—Er1—O6 | 77.85 (13) | C36—C37—H37 | 120.00 |
| O5—Er1—O7 | 76.12 (11) | C32—C37—H37 | 120.00 |
| O5—Er1—N1 | 130.59 (12) | N1—C41—H41 | 119.00 |
| O5—Er1—N2 | 154.27 (14) | C42—C41—H41 | 118.00 |
| O5—Er1—C21 | 27.81 (14) | C43—C42—H42 | 121.00 |
| O5—Er1—C31 | 73.95 (14) | C41—C42—H42 | 121.00 |
| O6—Er1—O7 | 54.37 (12) | C44—C43—H43 | 120.00 |
| O6—Er1—N1 | 142.83 (13) | C42—C43—H43 | 120.00 |
| O6—Er1—N2 | 96.83 (13) | C46—C45—H45 | 119.00 |
| O6—Er1—C21 | 102.45 (15) | C44—C45—H45 | 119.00 |
| O6—Er1—C31 | 27.09 (15) | C47—C46—H46 | 119.00 |
| O7—Er1—N1 | 143.43 (13) | C45—C46—H46 | 119.00 |
| O7—Er1—N2 | 80.37 (13) | C49—C48—H48 | 120.00 |
| O7—Er1—C21 | 100.89 (14) | C47—C48—H48 | 120.00 |
| O7—Er1—C31 | 27.34 (14) | C48—C49—H49 | 120.00 |
| N1—Er1—N2 | 67.14 (14) | C50—C49—H49 | 121.00 |
| N1—Er1—C21 | 102.79 (15) | C49—C50—H50 | 118.00 |
| N1—Er1—C31 | 155.46 (15) | N2—C50—H50 | 119.00 |
| N2—Er1—C21 | 157.08 (15) | C81$^{i}$—C81—C82 | 118.6 (6) |
| N2—Er1—C31 | 89.81 (15) | N7—C81—C82 | 122.5 (5) |
| C21—Er1—C31 | 101.75 (16) | N7—C81—C81$^{i}$ | 118.9 (6) |
| Er1—O1—N8 | 93.5 (3) | C82—C81—C86 | 122.5 (5) |
| Er1—O2—N8 | 98.0 (3) | N6—C81—C81$^{i}$ | 118.6 (6) |
| Er1—O4—C21 | 94.0 (3) | N6—C81—C86 | 122.5 (5) |
| Er1—O5—C21 | 92.0 (3) | C81$^{i}$—C81—C86 | 118.9 (6) |
| Er1—O6—C31 | 95.1 (3) | N6—C81—N7 | 122.5 (5) |
| Er1—O7—C31 | 91.8 (3) | C83—C82—C87 | 120.5 (8) |
| H3A—O3W—H3B | 110.00 | C81—C82—C83 | 116.7 (6) |
| Er1—O3W—H3B | 110.00 | C81—C82—C87 | 122.7 (8) |
| Er1—O3W—H3A | 118.00 | N6—C83—C84 | 122.4 (8) |
| C25—O8—H8 | 109.00 | C82—C83—C84 | 122.4 (8) |

| | | | |
|---|---|---|---|
| C35—O9—H9 | 109.00 | C83—C84—C85 | 119.4 (7) |
| H1A—O1W—H1B | 108.00 | C84—C85—C86 | 121.7 (8) |
| C41—N1—C52 | 117.8 (5) | N7—C85—C84 | 121.7 (8) |
| Er1—N1—C41 | 124.3 (3) | C81—C86—C85 | 117.4 (6) |
| Er1—N1—C52 | 117.7 (3) | C82—C87—C88 | 117.9 (13) |
| C50—N2—C51 | 117.7 (5) | N6—C87—C88 | 117.9 (13) |
| Er1—N2—C50 | 125.0 (4) | C82—C83—H83 | 119.00 |
| Er1—N2—C51 | 116.3 (3) | C84—C83—H83 | 119.00 |
| O1—N8—O2 | 115.5 (4) | N6—C83—H83 | 119.00 |
| O1—N8—O3 | 121.9 (5) | C85—C84—H84 | 120.00 |
| O2—N8—O3 | 122.5 (5) | C83—C84—H84 | 120.00 |
| H2A—O2W—H2B | 108.00 | C84—C85—H85 | 119.00 |
| C81—N6—C87 | 122.7 (8) | N7—C85—H85 | 119.00 |
| C81—N6—C83 | 116.7 (6) | C86—C85—H85 | 119.00 |
| C83—N6—C87 | 120.5 (8) | C88—C87—H87 | 121.00 |
| C81—N7—C85 | 117.4 (6) | N6—C87—H87 | 121.00 |
| C61—N3—C72 | 116.4 (8) | C82—C87—H87 | 121.00 |
| C70—N4—C71 | 120.9 (7) | C87—C88—H88 | 120.00 |
| C71—N4—H4 | 120.00 | N3—C61—C62 | 124.2 (9) |
| C70—N4—H4 | 119.00 | C61—C62—C63 | 119.4 (9) |
| O12—N5—O13 | 117.0 (11) | C62—C63—C64 | 119.3 (10) |
| O11—N5—O13 | 120.0 (11) | C63—C64—C65 | 123.3 (9) |
| O11—N5—O12 | 122.7 (12) | C63—C64—C72 | 117.6 (8) |
| Er1—C21—C22 | 177.2 (4) | C65—C64—C72 | 119.1 (7) |
| O4—C21—O5 | 119.1 (5) | C64—C65—C66 | 120.9 (9) |
| O4—C21—C22 | 120.6 (5) | C65—C66—C67 | 121.7 (10) |
| O5—C21—C22 | 120.3 (5) | C68—C67—C71 | 117.4 (9) |
| Er1—C21—O5 | 60.2 (3) | C66—C67—C71 | 118.9 (8) |
| Er1—C21—O4 | 59.0 (3) | C66—C67—C68 | 123.6 (9) |
| C21—C22—C27 | 120.9 (5) | C67—C68—C69 | 120.9 (9) |
| C23—C22—C27 | 119.1 (5) | C68—C69—C70 | 119.0 (8) |
| C21—C22—C23 | 120.0 (5) | N4—C70—C69 | 121.6 (9) |
| C22—C23—C24 | 120.1 (5) | N4—C71—C72 | 120.4 (6) |
| C23—C24—C25 | 121.1 (6) | C67—C71—C72 | 119.4 (7) |
| C24—C25—C26 | 119.0 (5) | N4—C71—C67 | 120.2 (6) |
| O8—C25—C24 | 118.0 (5) | N3—C72—C71 | 116.9 (6) |
| O8—C25—C26 | 123.1 (5) | C64—C72—C71 | 120.1 (6) |
| C25—C26—C27 | 120.5 (5) | N3—C72—C64 | 123.0 (6) |
| C22—C27—C26 | 120.2 (5) | N3—C61—H61 | 118.00 |
| Er1—C31—C32 | 174.6 (4) | C62—C61—H61 | 118.00 |
| Er1—C31—O6 | 57.9 (3) | C61—C62—H62 | 120.00 |
| O6—C31—C32 | 119.9 (5) | C63—C62—H62 | 120.00 |
| Er1—C31—O7 | 60.9 (3) | C64—C63—H63 | 120.00 |
| O7—C31—C32 | 121.6 (5) | C62—C63—H63 | 120.00 |
| O6—C31—O7 | 118.5 (5) | C66—C65—H65 | 120.00 |
| C33—C32—C37 | 118.7 (5) | C64—C65—H65 | 120.00 |
| C31—C32—C37 | 120.2 (6) | C65—C66—H66 | 119.00 |
| C31—C32—C33 | 121.1 (5) | C67—C66—H66 | 119.00 |
| C32—C33—C34 | 120.8 (5) | C67—C68—H68 | 120.00 |

| | | | |
|---|---|---|---|
| C33—C34—C35 | 119.7 (7) | C69—C68—H68 | 120.00 |
| C34—C35—C36 | 119.9 (7) | C70—C69—H69 | 120.00 |
| O9—C35—C36 | 117.9 (7) | C68—C69—H69 | 121.00 |
| O9—C35—C34 | 122.1 (7) | C69—C70—H70 | 119.00 |
| C35—C36—C37 | 120.0 (7) | N4—C70—H70 | 119.00 |
| C32—C37—C36 | 120.9 (7) | | |
| O2—Er1—O1—N8 | 4.8 (3) | Er1—O6—C31—O7 | 5.4 (5) |
| O3W—Er1—O1—N8 | 144.2 (3) | Er1—O6—C31—C32 | −174.3 (4) |
| O4—Er1—O1—N8 | 40.0 (3) | Er1—O7—C31—C32 | 174.4 (5) |
| O5—Er1—O1—N8 | −27.9 (4) | Er1—O7—C31—O6 | −5.2 (5) |
| O6—Er1—O1—N8 | −81.4 (3) | C52—N1—C41—C42 | 0.6 (8) |
| O7—Er1—O1—N8 | −117.7 (3) | Er1—N1—C52—C44 | −172.0 (4) |
| N1—Er1—O1—N8 | 101.0 (3) | Er1—N1—C52—C51 | 9.3 (6) |
| N2—Er1—O1—N8 | 172.7 (3) | C41—N1—C52—C44 | 2.4 (8) |
| C21—Er1—O1—N8 | 8.7 (4) | Er1—N1—C41—C42 | 174.6 (4) |
| C31—Er1—O1—N8 | −98.2 (3) | C41—N1—C52—C51 | −176.4 (5) |
| O1—Er1—O2—N8 | −4.8 (3) | C50—N2—C51—C47 | −1.6 (8) |
| O3W—Er1—O2—N8 | −140.2 (3) | C50—N2—C51—C52 | 175.3 (5) |
| O4—Er1—O2—N8 | −154.0 (3) | Er1—N2—C51—C52 | −15.8 (6) |
| O5—Er1—O2—N8 | 150.7 (3) | Er1—N2—C50—C49 | −165.8 (4) |
| O6—Er1—O2—N8 | 71.6 (3) | C51—N2—C50—C49 | 2.1 (8) |
| O7—Er1—O2—N8 | 84.1 (3) | Er1—N2—C51—C47 | 167.3 (4) |
| N1—Er1—O2—N8 | −77.2 (3) | C83—N6—C87—C88 | −179.0 (12) |
| N2—Er1—O2—N8 | −17.8 (3) | C83—N6—C81—C86 | 0.4 (11) |
| C21—Er1—O2—N8 | 178.3 (3) | C83—N6—C81—C81$^{i}$ | 179.9 (7) |
| C31—Er1—O2—N8 | 78.6 (3) | C87—N6—C81—N7 | 177.0 (9) |
| O1—Er1—O4—C21 | −118.5 (3) | C87—N6—C81—C86 | 177.0 (9) |
| O2—Er1—O4—C21 | −90.4 (3) | C87—N6—C81—C81$^{i}$ | −3.4 (12) |
| O3W—Er1—O4—C21 | 97.3 (3) | C81—N6—C83—C84 | 0.5 (12) |
| O5—Er1—O4—C21 | 1.7 (3) | C83—N6—C81—N7 | 0.4 (11) |
| O6—Er1—O4—C21 | −31.3 (4) | C81—N6—C87—C88 | 4.5 (18) |
| O7—Er1—O4—C21 | 36.4 (3) | C87—N6—C83—C84 | −176.3 (10) |
| N1—Er1—O4—C21 | −177.9 (3) | C85—N7—C81—C81$^{i}$ | 179.6 (7) |
| N2—Er1—O4—C21 | 150.9 (3) | C81—N7—C85—C84 | 0.5 (12) |
| C31—Er1—O4—C21 | 2.9 (4) | C85—N7—C81—C82 | −0.8 (11) |
| O1—Er1—O5—C21 | 101.0 (3) | C85—N7—C81—N6 | −0.8 (11) |
| O2—Er1—O5—C21 | 75.6 (3) | C61—N3—C72—C64 | −2.2 (11) |
| O3W—Er1—O5—C21 | −74.4 (3) | C72—N3—C61—C62 | −0.2 (12) |
| O4—Er1—O5—C21 | −1.6 (3) | C61—N3—C72—C71 | 177.9 (7) |
| O6—Er1—O5—C21 | 151.8 (3) | C71—N4—C70—C69 | −0.8 (12) |
| O7—Er1—O5—C21 | −152.4 (3) | C70—N4—C71—C67 | −0.2 (11) |
| N1—Er1—O5—C21 | −1.0 (4) | C70—N4—C71—C72 | −178.6 (7) |
| N2—Er1—O5—C21 | −127.8 (4) | O5—C21—C22—C23 | −179.2 (5) |
| C31—Er1—O5—C21 | 179.4 (3) | O4—C21—C22—C27 | −176.5 (5) |
| O1—Er1—O6—C31 | −140.4 (3) | O5—C21—C22—C27 | 3.2 (8) |
| O2—Er1—O6—C31 | 164.8 (3) | O4—C21—C22—C23 | 1.2 (8) |
| O3W—Er1—O6—C31 | 6.7 (4) | C21—C22—C23—C24 | −177.9 (6) |
| O4—Er1—O6—C31 | 105.5 (3) | C23—C22—C27—C26 | 0.2 (9) |

| | | | |
|---|---|---|---|
| O5—Er1—O6—C31 | 78.5 (3) | C21—C22—C27—C26 | 177.9 (5) |
| O7—Er1—O6—C31 | −3.1 (3) | C27—C22—C23—C24 | −0.2 (9) |
| N1—Er1—O6—C31 | −136.7 (3) | C22—C23—C24—C25 | −0.3 (9) |
| N2—Er1—O6—C31 | −76.0 (3) | C23—C24—C25—C26 | 0.8 (9) |
| C21—Er1—O6—C31 | 91.5 (3) | C23—C24—C25—O8 | −179.0 (6) |
| O1—Er1—O7—C31 | 46.4 (3) | O8—C25—C26—C27 | 179.0 (5) |
| O2—Er1—O7—C31 | −11.9 (3) | C24—C25—C26—C27 | −0.8 (9) |
| O3W—Er1—O7—C31 | −169.4 (3) | C25—C26—C27—C22 | 0.3 (9) |
| O4—Er1—O7—C31 | −110.5 (3) | O6—C31—C32—C37 | 2.9 (8) |
| O5—Er1—O7—C31 | −81.8 (3) | O6—C31—C32—C33 | −176.3 (5) |
| O6—Er1—O7—C31 | 3.0 (3) | O7—C31—C32—C33 | 4.1 (8) |
| N1—Er1—O7—C31 | 135.8 (3) | O7—C31—C32—C37 | −176.7 (5) |
| N2—Er1—O7—C31 | 108.7 (3) | C31—C32—C33—C34 | 178.5 (5) |
| C21—Er1—O7—C31 | −94.6 (3) | C33—C32—C37—C36 | 0.2 (9) |
| O1—Er1—N1—C41 | −112.5 (4) | C31—C32—C37—C36 | −179.1 (6) |
| O1—Er1—N1—C52 | 61.5 (4) | C37—C32—C33—C34 | −0.8 (8) |
| O2—Er1—N1—C41 | −60.2 (4) | C32—C33—C34—C35 | 0.6 (9) |
| O2—Er1—N1—C52 | 113.7 (4) | C33—C34—C35—O9 | −177.7 (7) |
| O3W—Er1—N1—C41 | 91.0 (4) | C33—C34—C35—C36 | 0.3 (11) |
| O3W—Er1—N1—C52 | −95.0 (4) | O9—C35—C36—C37 | 177.2 (7) |
| O4—Er1—N1—C41 | 16.6 (4) | C34—C35—C36—C37 | −0.8 (12) |
| O4—Er1—N1—C52 | −169.5 (4) | C35—C36—C37—C32 | 0.6 (11) |
| O5—Er1—N1—C41 | 16.0 (5) | N1—C41—C42—C43 | −2.0 (9) |
| O5—Er1—N1—C52 | −170.0 (3) | C41—C42—C43—C44 | 0.4 (9) |
| O6—Er1—N1—C41 | −116.2 (4) | C42—C43—C44—C45 | −178.3 (6) |
| O6—Er1—N1—C52 | 57.8 (5) | C42—C43—C44—C52 | 2.3 (8) |
| O7—Er1—N1—C41 | 144.7 (4) | C43—C44—C52—C51 | 174.9 (5) |
| O7—Er1—N1—C52 | −41.4 (5) | C45—C44—C52—C51 | −4.5 (8) |
| N2—Er1—N1—C41 | 173.9 (5) | C45—C44—C52—N1 | 176.7 (5) |
| N2—Er1—N1—C52 | −12.2 (4) | C43—C44—C45—C46 | −177.6 (6) |
| C21—Er1—N1—C41 | 15.6 (4) | C43—C44—C52—N1 | −3.8 (8) |
| C21—Er1—N1—C52 | −170.5 (4) | C52—C44—C45—C46 | 1.9 (9) |
| C31—Er1—N1—C41 | −164.9 (4) | C44—C45—C46—C47 | 2.7 (10) |
| C31—Er1—N1—C52 | 9.0 (6) | C45—C46—C47—C51 | −4.5 (9) |
| O1—Er1—N2—C50 | 103.0 (4) | C45—C46—C47—C48 | 175.1 (6) |
| O1—Er1—N2—C51 | −65.0 (4) | C48—C47—C51—C52 | −178.0 (5) |
| O2—Er1—N2—C50 | 114.1 (4) | C46—C47—C51—N2 | 178.4 (5) |
| O2—Er1—N2—C51 | −53.9 (4) | C46—C47—C48—C49 | −176.1 (6) |
| O3W—Er1—N2—C50 | −93.2 (4) | C51—C47—C48—C49 | 3.5 (9) |
| O3W—Er1—N2—C51 | 98.9 (4) | C46—C47—C51—C52 | 1.6 (8) |
| O4—Er1—N2—C50 | −144.6 (4) | C48—C47—C51—N2 | −1.1 (9) |
| O4—Er1—N2—C51 | 47.5 (4) | C47—C48—C49—C50 | −3.0 (9) |
| O5—Er1—N2—C50 | −38.9 (6) | C48—C49—C50—N2 | 0.2 (9) |
| O5—Er1—N2—C51 | 153.2 (3) | N2—C51—C52—N1 | 4.6 (8) |
| O6—Er1—N2—C50 | 37.3 (4) | N2—C51—C52—C44 | −174.2 (5) |
| O6—Er1—N2—C51 | −130.7 (4) | C47—C51—C52—C44 | 2.8 (8) |
| O7—Er1—N2—C50 | −14.8 (4) | C47—C51—C52—N1 | −178.4 (5) |
| O7—Er1—N2—C51 | 177.3 (4) | C86—C81—C82—C83 | 0.4 (11) |
| N1—Er1—N2—C50 | −177.6 (5) | C86—C81—C82—C87 | 177.0 (9) |

| | | | |
|---|---|---|---|
| N1—Er1—N2—C51 | 14.4 (3) | N7—C81—C82—C87 | 177.0 (9) |
| C21—Er1—N2—C50 | −110.0 (5) | N6—C81—C81$^{i}$—N6$^{i}$ | −180.0 (7) |
| C21—Er1—N2—C51 | 82.1 (6) | N6—C81—C81$^{i}$—N7$^{i}$ | 0.4 (10) |
| C31—Er1—N2—C50 | 11.0 (4) | C81$^{i}$—C81—C82—C83 | 179.9 (7) |
| C31—Er1—N2—C51 | −156.9 (4) | C81$^{i}$—C81—C82—C87 | −3.4 (12) |
| O1—Er1—C21—O4 | 79.9 (3) | N6—C81—C86—C85 | −0.8 (11) |
| O1—Er1—C21—O5 | −103.0 (3) | C82—C81—C86—C85 | −0.8 (11) |
| O2—Er1—C21—O4 | 83.1 (3) | C81$^{i}$—C81—C86—C85 | 179.6 (7) |
| O2—Er1—C21—O5 | −99.8 (3) | C86—C81—C81$^{i}$—N7$^{i}$ | −180.0 (7) |
| O3W—Er1—C21—O4 | −75.7 (3) | N7—C81—C82—C83 | 0.4 (11) |
| O3W—Er1—C21—O5 | 101.4 (3) | C82—C81—C81$^{i}$—N6$^{i}$ | −180.0 (7) |
| O4—Er1—C21—O5 | 177.1 (5) | N7—C81—C81$^{i}$—N6$^{i}$ | −0.4 (10) |
| O5—Er1—C21—O4 | −177.1 (5) | N7—C81—C81$^{i}$—N7$^{i}$ | −180.0 (7) |
| O6—Er1—C21—O4 | 154.6 (3) | C82—C81—C81$^{i}$—N7$^{i}$ | 0.4 (10) |
| O6—Er1—C21—O5 | −28.3 (3) | C86—C81—C81$^{i}$—N6$^{i}$ | −0.4 (10) |
| O7—Er1—C21—O4 | −149.8 (3) | C87—C82—C83—C84 | −176.3 (10) |
| O7—Er1—C21—O5 | 27.3 (3) | C81—C82—C83—C84 | 0.5 (12) |
| N1—Er1—C21—O4 | 2.1 (3) | C81—C82—C87—C88 | 4.5 (18) |
| N1—Er1—C21—O5 | 179.2 (3) | C83—C82—C87—C88 | −179.0 (12) |
| N2—Er1—C21—O4 | −58.8 (6) | N6—C83—C84—C85 | −0.8 (14) |
| N2—Er1—C21—O5 | 118.3 (4) | C82—C83—C84—C85 | −0.8 (14) |
| C31—Er1—C21—O4 | −177.7 (3) | C83—C84—C85—C86 | 0.3 (14) |
| C31—Er1—C21—O5 | −0.6 (3) | C83—C84—C85—N7 | 0.3 (14) |
| O1—Er1—C31—O6 | 36.9 (3) | C84—C85—C86—C81 | 0.5 (12) |
| O1—Er1—C31—O7 | −137.7 (3) | N3—C61—C62—C63 | 1.9 (14) |
| O2—Er1—C31—O6 | −15.0 (3) | C61—C62—C63—C64 | −1.1 (13) |
| O2—Er1—C31—O7 | 170.5 (3) | C62—C63—C64—C65 | 179.8 (9) |
| O3W—Er1—C31—O6 | −174.8 (3) | C62—C63—C64—C72 | −1.1 (12) |
| O3W—Er1—C31—O7 | 10.6 (3) | C63—C64—C65—C66 | 177.9 (9) |
| O4—Er1—C31—O6 | −95.8 (3) | C72—C64—C65—C66 | −1.2 (13) |
| O4—Er1—C31—O7 | 89.7 (3) | C63—C64—C72—N3 | 2.9 (11) |
| O5—Er1—C31—O6 | −94.7 (3) | C63—C64—C72—C71 | −177.3 (7) |
| O5—Er1—C31—O7 | 90.7 (3) | C65—C64—C72—N3 | −178.0 (7) |
| O6—Er1—C31—O7 | −174.6 (5) | C65—C64—C72—C71 | 1.9 (11) |
| O7—Er1—C31—O6 | 174.6 (5) | C64—C65—C66—C67 | 0.2 (15) |
| N1—Er1—C31—O6 | 86.1 (5) | C65—C66—C67—C68 | −178.3 (10) |
| N1—Er1—C31—O7 | −88.5 (5) | C65—C66—C67—C71 | 0.1 (14) |
| N2—Er1—C31—O6 | 105.5 (3) | C66—C67—C68—C69 | 178.4 (10) |
| N2—Er1—C31—O7 | −69.1 (3) | C71—C67—C68—C69 | 0.0 (14) |
| C21—Er1—C31—O6 | −94.4 (3) | C66—C67—C71—N4 | −177.9 (8) |
| C21—Er1—C31—O7 | 91.0 (3) | C66—C67—C71—C72 | 0.5 (11) |
| Er1—O1—N8—O3 | 173.3 (5) | C68—C67—C71—N4 | 0.6 (11) |
| Er1—O1—N8—O2 | −7.9 (4) | C68—C67—C71—C72 | 179.0 (8) |
| Er1—O2—N8—O3 | −173.0 (5) | C67—C68—C69—C70 | −0.9 (15) |
| Er1—O2—N8—O1 | 8.3 (5) | C68—C69—C70—N4 | 1.3 (14) |
| Er1—O4—C21—O5 | −2.9 (5) | N4—C71—C72—N3 | −3.3 (10) |
| Er1—O4—C21—C22 | 176.8 (5) | N4—C71—C72—C64 | 176.9 (7) |

| | | | |
|---|---|---|---|
| Er1—O5—C21—C22 | −176.8 (5) | C67—C71—C72—N3 | 178.3 (7) |
| Er1—O5—C21—O4 | 2.9 (5) | C67—C71—C72—C64 | −1.5 (10) |

Symmetry codes: (i) −*x*+2, −*y*, −*z*+1.

*Hydrogen-bond geometry (Å, °)*

Cg4 is the centroid of the C32–C37 ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1W—H1A···O2$^{ii}$ | 0.82 | 2.55 | 3.270 (6) | 148 |
| O1W—H1A···O6$^{ii}$ | 0.82 | 2.22 | 2.875 (6) | 137 |
| O1W—H1B···O12$^{ii}$ | 0.82 | 2.06 | 2.872 (10) | 172 |
| O2W—H2A···O9$^{iii}$ | 0.82 | 1.94 | 2.737 (8) | 164 |
| O2W—H2B···O11$^{ii}$ | 0.82 | 2.01 | 2.789 (10) | 157 |
| O3W—H3A···O5$^{iv}$ | 0.82 | 1.90 | 2.671 (5) | 155 |
| O3W—H3B···O7$^{iv}$ | 0.82 | 2.16 | 2.836 (5) | 140 |
| N4—H4···O2W | 0.86 | 1.91 | 2.725 (9) | 157 |
| O8—H8···O1W$^{v}$ | 0.82 | 1.87 | 2.659 (6) | 160 |
| O9—H9···O11$^{vi}$ | 0.82 | 2.09 | 2.803 (12) | 145 |
| O9—H9···O12$^{vi}$ | 0.82 | 2.43 | 3.172 (12) | 151 |
| C34—H34···O3$^{vi}$ | 0.93 | 2.43 | 3.256 (8) | 148 |
| C48—H48···O12$^{vii}$ | 0.93 | 2.27 | 3.046 (11) | 141 |
| C62—H62···O1$^{viii}$ | 0.93 | 2.55 | 3.387 (10) | 150 |
| C70—H70···O13$^{ii}$ | 0.93 | 2.35 | 3.244 (13) | 161 |
| C83—H83···Cg4$^{iii}$ | 0.93 | 2.78 | 3.628 (9) | 152 |

Symmetry codes: (ii) −*x*+1, −*y*+1, −*z*+1; (iii) *x*+1, *y*, *z*; (iv) −*x*, −*y*+1, −*z*; (v) *x*−1, *y*+1, *z*−1; (vi) *x*−1, *y*, *z*; (vii) *x*, *y*−1, *z*; (viii) *x*, *y*+1, *z*.

**Fig. 1**

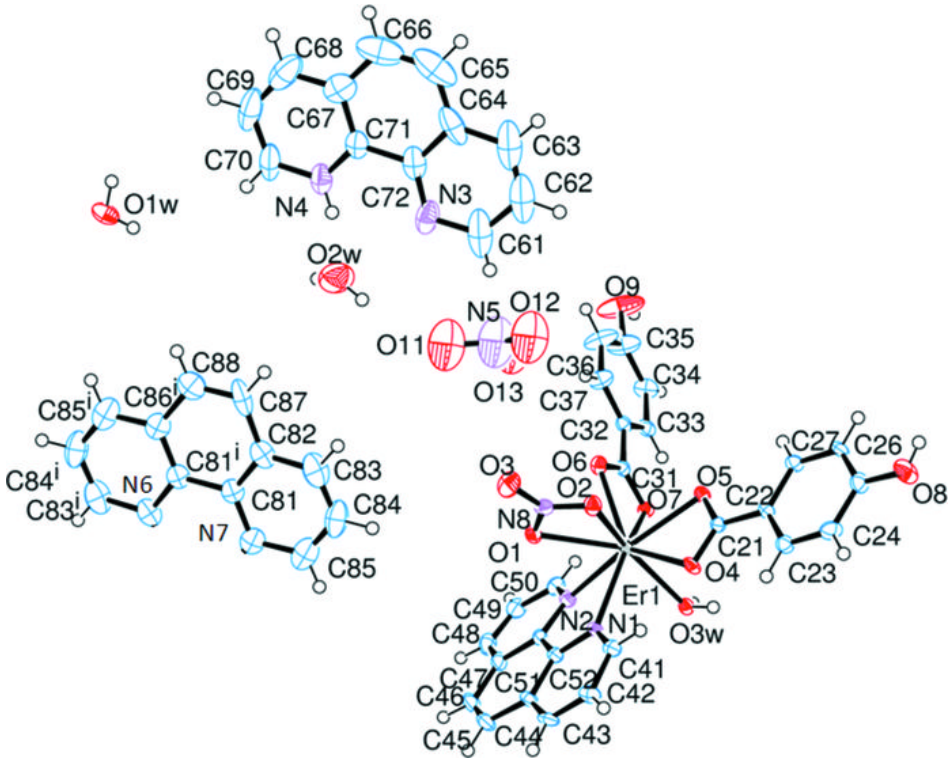
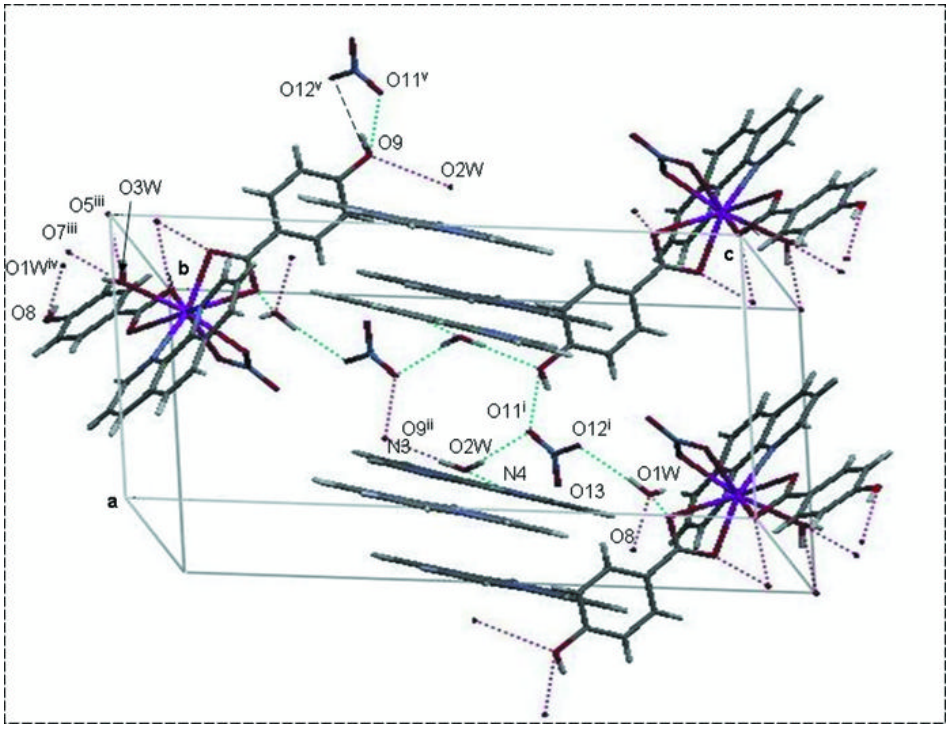

C66
C68
C65
C69
C64
C67
C71
C63
C70
C62
O1w
N4
C72
N3
C61
O2w
O9
N5
O12
C35
O11
C36
C34
O13
C37
C33
C88
C32
C87
C85i
C86i
C82
C27
C26
C84i
C81i
C83
O3
O6
C31
O5
O8
N6
O2
O7
C22
C83i
C81
C84
N8
C24
N7
O1
C21
C85
O4
C23
C50
Er1
C49
N2
N1
O3w
C48
C41
C47
C51
C52
C42
C46
C45
C44
C43

**Fig. 2**


O12v
O11v
O9
O2W
O3W
O5iii
O7iii
O1Wiv
O8
b
c
a
O11i
O12i
O9ii
N3
O2W
N4
O13
O1W
O8