

## Poly[[tetraquatetrakis[ $\mu_3$ -5-(pyridine-4-carboxamido)isophthalato]cobalt(II)-dierbium(III)] tetrahydrate]

Yi-Fang Deng, Man-Sheng Chen,\* Chun-Hua Zhang\* and Xiong-Wen Tan

Key Laboratory of Functional Organometallic Materials, Hengyang Normal University, Department of Chemistry and Materials Science, Hengyang, Hunan 421008, People's Republic of China  
Correspondence e-mail: cmsniu@163.com, zhangchunhua668@163.com

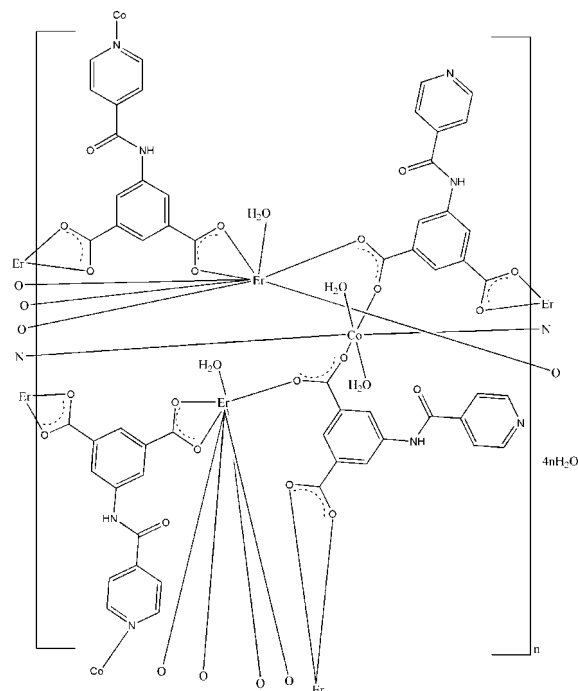
Received 20 September 2011; accepted 28 September 2011

Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.009$  Å;  $R$  factor = 0.052;  $wR$  factor = 0.136; data-to-parameter ratio = 11.6.

In the centrosymmetric polymeric title compound,  $\{[\text{CoEr}_2(\text{C}_{14}\text{H}_8\text{N}_2\text{O}_5)_4(\text{H}_2\text{O})_4] \cdot 4\text{H}_2\text{O}\}_n$ , the  $\text{Er}^{\text{III}}$  cation has a coordination number of eight and is surrounded by seven carboxylate O atoms from four 5-(pyridine-4-carboxamido)-isophthalate (*L*) ligands and one water molecule, forming a distorted square-antiprismatic arrangement. The  $\text{Co}^{\text{II}}$  cation is located on an inversion center and is coordinated by two pyridine N atoms, two carboxylate O atoms and two water molecules in a distorted octahedral geometry. The asymmetric unit contains two anionic *L* ligands. One bridges two  $\text{Er}^{\text{III}}$  cations and one  $\text{Co}^{\text{II}}$  cation through two carboxylate groups and one pyridine N atom, while the other bridges two  $\text{Er}^{\text{III}}$  cations and one  $\text{Co}^{\text{II}}$  cation through two carboxylate groups. Extensive  $\text{O}-\text{H}\cdots\text{O}$ ,  $\text{O}-\text{H}\cdots\text{N}$  and  $\text{N}-\text{H}\cdots\text{O}$  hydrogen-bonding interactions are present in the crystal, involving all uncoordinated water molecules and the uncoordinated pyridine N atom of one of the ligands bonded to an adjacent coordinated water molecule. The title compound is isotypic with the gadolinium analogue.

### Related literature

For the isotypic structure of the gadolinium analogue, see: Deng *et al.* (2011). For related hetero-metallic complexes, see: Chen *et al.* (2011*a,b*); Gu & Xue (2006); Liang *et al.* (2000); Prasad *et al.* (2007); Zhao *et al.* (2003, 2004).



### Experimental

#### Crystal data

$[\text{CoEr}_2(\text{C}_{14}\text{H}_8\text{N}_2\text{O}_5)_4(\text{H}_2\text{O})_4] \cdot 4\text{H}_2\text{O}$   
 $M_r = 1674.47$   
Triclinic,  $P\bar{1}$   
 $a = 10.0816$  (9) Å  
 $b = 10.7844$  (10) Å  
 $c = 13.7316$  (12) Å  
 $\alpha = 79.174$  (1)°  
 $\beta = 78.771$  (2)°

$\gamma = 86.355$  (2)°  
 $V = 1437.7$  (2) Å<sup>3</sup>  
 $Z = 1$   
Mo  $K\alpha$  radiation  
 $\mu = 3.28$  mm<sup>-1</sup>  
 $T = 293$  K  
0.20 × 0.18 × 0.10 mm

#### Data collection

Bruker SMART CCD area-detector diffractometer  
Absorption correction: multi-scan (SADABS; Bruker, 2000)  
 $T_{\text{min}} = 0.560$ ,  $T_{\text{max}} = 0.735$   
7172 measured reflections  
4979 independent reflections  
4649 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.096$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.052$   
 $wR(F^2) = 0.136$   
 $S = 1.02$   
4979 reflections

430 parameters  
H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 3.52$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -2.99$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1}-\text{H1}\cdots\text{O3W}^{\text{i}}$	0.86	2.16	3.007 (8)	166
$\text{O1W}-\text{H1WB}\cdots\text{O4W}^{\text{ii}}$	0.85	2.05	2.769 (9)	142
$\text{O1W}-\text{H1WA}\cdots\text{O8}^{\text{iii}}$	0.85	2.22	2.975 (8)	149
$\text{O2W}-\text{H2WB}\cdots\text{O4W}^{\text{iv}}$	0.85	2.32	3.109 (10)	156
$\text{O2W}-\text{H2WC}\cdots\text{N2}^{\text{v}}$	0.85	1.94	2.687 (8)	147
$\text{O3W}-\text{H3WA}\cdots\text{O7}^{\text{vi}}$	0.85	2.30	3.041 (8)	147
$\text{O3W}-\text{H3WB}\cdots\text{O9}$	0.85	2.30	3.042 (8)	147
$\text{O4W}-\text{H4WA}\cdots\text{O3}^{\text{vii}}$	0.85	1.92	2.729 (8)	159
$\text{O4W}-\text{H4WB}\cdots\text{O6}^{\text{viii}}$	0.85	1.95	2.762 (8)	159

Symmetry codes: (i)  $x-1, y, z$ ; (ii)  $x-1, y, z+1$ ; (iii)  $-x, -y+1, -z+2$ ; (iv)  $x-1, y+1, z+1$ ; (v)  $x, y, z+1$ ; (vi)  $x+1, y, z$ ; (vii)  $x+1, y, z-1$ ; (viii)  $-x+1, -y+1, -z+1$ .

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINTE* (Bruker, 2000); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *XP* in *SHELXTL* and *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXTL*.

This work was supported by the Open Fund Project of Key Laboratory in Hunan Universities (11 K009) and the Science Foundation of Hengyang Normal University of China (10B67).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2536).

## References

- Brandenburg, K. (1999). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
- Bruker (2000). *SMART*, *SAINTE* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Chen, M. S., Deng, Y. F., Zhang, C. H., Kang, D. Z., Nie, X. & Liu, Y. (2011a). *Inorg. Chem. Commun.* **14**, 944–947.
- Chen, M. S., Zhao, Y., Okamura, T.-A., Su, Z., Sun, W. Y. & Ueyama, N. (2011b). *Supramol. Chem.* **23**, 117–124.
- Deng, Y.-F., Chen, M.-S., Zhang, C.-H. & Kuang, D.-Z. (2011). *Acta Cryst.* **E67**, m1431–m1432.
- Gu, X. J. & Xue, D. F. (2006). *Inorg. Chem.* **45**, 9257–9261.
- Liang, Y. C., Cao, R., Su, W. P., Hong, M. C. & Zhang, W. J. (2000). *Angew. Chem. Int. Ed.* **39**, 3304–3307.
- Prasad, T. K., Rajasekharan, M. V. & Costes, J. P. (2007). *Angew. Chem. Int. Ed.* **46**, 2851–2854.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Zhao, B., Cheng, P., Chen, X. Y., Cheng, C., Shi, W., Liao, D. Z., Yan, S. P. & Jiang, Z. H. (2004). *J. Am. Chem. Soc.* **126**, 3012–3013.
- Zhao, B., Cheng, P., Dai, Y., Cheng, C., Liao, D. Z., Yan, S. P., Jiang, Z. H. & Wang, G. L. (2003). *Angew. Chem. Int. Ed.* **42**, 934–936.

**supplementary materials**

*Acta Cryst.* (2011). E67, m1478-m1479 [ doi:10.1107/S1600536811039948 ]

## Poly[[tetraaquatetrakis[ $\mu_3$ -5-(pyridine-4-carboxamido)isophthalato]cobalt(II)dierbium(III)] tetrahydrate]

Y.-F. Deng, M.-S. Chen, C.-H. Zhang and X.-W. Tan

### Comment

The rational design and synthesis of higher-dimensional transition-lanthanide metal heterometallic networks have attracted increasing attention, which is justified not only by the fascinating structural diversity of the resulting architectures but also by the potential applications of these complexes as important functional solid materials (Chen *et al.*, 2011*a,b*; Gu & Xue, 2006; Liang *et al.*, 2000; Prasad *et al.*, 2007; Zhao *et al.*, 2003, 2004). In this context, we have synthesized a new *3d-4f* coordination polymer,  $[\text{CoEr}_2(\text{C}_{14}\text{H}_8\text{O}_5\text{N}_2)_4(\text{H}_2\text{O})_4]\cdot 4\text{H}_2\text{O}$ , or  $[\text{CoEr}_2(L)_4(\text{H}_2\text{O})_4]\cdot 4\text{H}_2\text{O}$  and report its crystal structure here.

The title compound is isotopic with the gadolinium analogue (Deng *et al.*, 2011). The central  $\text{Er}^{\text{III}}$  ion is eight-coordinated by seven O atoms from four  $L^{2-}$  ligands and one water molecule, forming a distorted square antiprismatic arrangement around the metal (Fig. 1). The carboxyl groups of the two unique  $L^{2-}$  ligands exhibit different coordination modes: one coordinates to two  $\text{Er}^{\text{III}}$  and one  $\text{Co}^{\text{II}}$  atom (site symmetry  $\bar{1}$ ) using its two carboxylate groups with bidentate-chelate and bis-monodentate coordination modes while the pyridyl group is free of coordination. The other ligand coordinates to two  $\text{Er}^{\text{III}}$  ions through the carboxylate groups with a bidentate-chelate coordination mode and to one  $\text{Co}^{\text{II}}$  *via* the pyridyl group. Based on the coordination modes of the carboxylate and pyridyl groups of the ligands, a three-dimensional network is formed (Fig. 2), which is similar to that of complexes of the type  $\{[\text{LnCo}_{0.5}(\text{INAIP})_2(\text{H}_2\text{O})_2]\cdot 2\text{H}_2\text{O}\}_n$  (Chen, *et al.* 2011*b*). Extensive O—H $\cdots$ O and N—H $\cdots$ O hydrogen bonding interactions are present in the crystal structure (Table 1).

### Experimental

A mixture of 0.05 mmol  $\text{Er}(\text{NO}_3)_3\cdot 6\text{H}_2\text{O}$  (22.5 mg, 0.05 mmol),  $\text{H}_2L$  (28.6 mg, 0.1 mmol),  $\text{Co}(\text{OAc})_2\cdot 4\text{H}_2\text{O}$  (13.2 mg, 0.05 mmol), NaOH (6.0 mg, 0.15 mmol), MeOH (4 ml) and  $\text{H}_2\text{O}$  (6 ml) was heated in a 16 mL capacity Teflon-lined reaction vessel at 433 K for 4 days. The reaction mixture was then cooled to room temperature over a period of 40 h. The product was collected by filtration, washed with water and air-dried.

### Refinement

H atoms bonded to C atoms were placed geometrically and refined as riding atoms. The pyridyl N atoms were found from a difference Fourier maps and refined as riding, with N—H = 0.8600 Å, and the water H atoms were found from Fourier difference maps and refined with restraints for O—H distances (0.85 Å) with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{O})$ . The highest residual electron density was found at 0.88 Å from Er1 atom and the deepest hole at 0.91 Å from the Er1 atom.

Figures

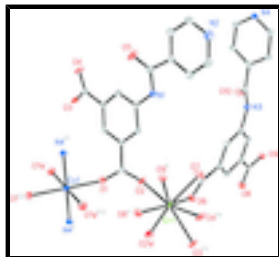


Fig. 1. The ORTEP drawing of the title compound (I). Displacement ellipsoids are drawn at the 30% probability level. [Symmetry codes: (i)  $-1 + x, y, 1 + z$  (ii)  $-x, 1 - y, 1 - z$  (iii)  $-1 - x, 1 - y, 2 - z$  (iv)  $x, 1 + y, z$  (v)  $-1 + x, y, z$ .]

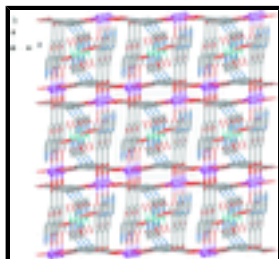


Fig. 2. Projection along [001] showing the three-dimensional structure of the compound. Colour code: Er (pink), Co (light blue), O (red), N (blue), C (grey).

**Poly[[tetraaquatetrakis[ $\mu_3$ -5-(pyridine-4-carboxamido)isophthalato]cobalt(II)dierbium(III)] tetrahydrate]**

*Crystal data*

[CoEr<sub>2</sub>(C<sub>14</sub>H<sub>8</sub>N<sub>2</sub>O<sub>5</sub>)<sub>4</sub>(H<sub>2</sub>O)<sub>4</sub>] $\cdot$ 4H<sub>2</sub>O

$M_r = 1674.47$

Triclinic,  $P\bar{1}$

Hall symbol:  $-P\ 1$

$a = 10.0816$  (9) Å

$b = 10.7844$  (10) Å

$c = 13.7316$  (12) Å

$\alpha = 79.174$  (1)°

$\beta = 78.771$  (2)°

$\gamma = 86.355$  (2)°

$V = 1437.7$  (2) Å<sup>3</sup>

$Z = 1$

$F(000) = 827$

$D_x = 1.934$  Mg m<sup>-3</sup>

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

Cell parameters from 5230 reflections

$\theta = 2.3$ – $28.1$ °

$\mu = 3.28$  mm<sup>-1</sup>

$T = 293$  K

Block, pink

$0.20 \times 0.18 \times 0.10$  mm

*Data collection*

Bruker SMART CCD area-detector diffractometer

4979 independent reflections

Radiation source: fine-focus sealed tube graphite

4649 reflections with  $I > 2\sigma(I)$

$\phi$  and  $\omega$  scans

$R_{int} = 0.096$

$\theta_{max} = 25.0$ °,  $\theta_{min} = 1.9$ °

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

$h = -5$ → $12$

$T_{min} = 0.560$ ,  $T_{max} = 0.735$

$k = -12$ → $12$

7172 measured reflections

$l = -15$ → $16$

Refinement

Refinement on $F^2$	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.052$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.136$	H-atom parameters constrained
$S = 1.02$	$w = 1/[\sigma^2(F_o^2) + (0.1058P)^2]$
4979 reflections	where $P = (F_o^2 + 2F_c^2)/3$
430 parameters	$(\Delta/\sigma)_{\max} = 0.001$
0 restraints	$\Delta\rho_{\max} = 3.52 \text{ e } \text{\AA}^{-3}$
	$\Delta\rho_{\min} = -2.99 \text{ e } \text{\AA}^{-3}$

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 ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	-0.5000	0.5000	1.0000	0.0223 (3)
Er1	-0.18176 (2)	0.92224 (2)	0.796262 (18)	0.01355 (14)
C1	-0.2010 (6)	0.5274 (6)	0.7723 (5)	0.0162 (12)
C2	-0.1777 (7)	0.5835 (6)	0.6709 (5)	0.0203 (13)
H2A	-0.1712	0.6707	0.6528	0.024*
C3	-0.1640 (6)	0.5091 (6)	0.5959 (5)	0.0178 (13)
C4	-0.1655 (6)	0.3777 (6)	0.6249 (5)	0.0187 (13)
H4A	-0.1543	0.3266	0.5762	0.022*
C5	-0.1833 (6)	0.3243 (6)	0.7250 (5)	0.0165 (12)
C6	-0.2041 (6)	0.3972 (6)	0.8004 (5)	0.0187 (13)
H6A	-0.2197	0.3594	0.8682	0.022*
C7	-0.1869 (6)	0.1837 (6)	0.7518 (5)	0.0178 (13)
C8	-0.2318 (7)	0.6074 (6)	0.8526 (5)	0.0205 (14)
C9	-0.1651 (7)	0.5169 (7)	0.4170 (5)	0.0264 (15)
C10	-0.1506 (7)	0.6000 (7)	0.3142 (5)	0.0239 (15)
C11	-0.1432 (8)	0.5403 (8)	0.2318 (5)	0.0325 (17)
H11A	-0.1416	0.4526	0.2406	0.039*
C12	-0.1385 (9)	0.6116 (8)	0.1383 (5)	0.0356 (18)

## supplementary materials

---

H12A	-0.1338	0.5698	0.0843	0.043*
C13	-0.1448 (8)	0.7939 (8)	0.1996 (6)	0.0337 (17)
H13A	-0.1442	0.8816	0.1888	0.040*
C14	-0.1505 (8)	0.7294 (7)	0.2963 (5)	0.0284 (16)
H14A	-0.1543	0.7730	0.3491	0.034*
C15	0.2360 (7)	0.8871 (6)	0.6690 (5)	0.0198 (14)
C16	0.2649 (6)	0.8586 (6)	0.5711 (5)	0.0188 (13)
H16A	0.1946	0.8527	0.5375	0.023*
C17	0.3943 (6)	0.8397 (6)	0.5257 (5)	0.0182 (13)
C18	0.5006 (6)	0.8521 (6)	0.5738 (5)	0.0192 (13)
H18A	0.5896	0.8420	0.5413	0.023*
C19	0.4738 (6)	0.8796 (6)	0.6698 (5)	0.0191 (13)
C20	0.3414 (6)	0.8968 (6)	0.7185 (5)	0.0199 (13)
H20A	0.3237	0.9147	0.7835	0.024*
C21	0.0908 (6)	0.9019 (6)	0.7170 (5)	0.0195 (13)
C22	0.5927 (6)	0.8916 (6)	0.7177 (5)	0.0181 (13)
C23	0.5058 (6)	0.7065 (7)	0.4098 (5)	0.0211 (14)
C24	0.5094 (6)	0.6636 (7)	0.3100 (5)	0.0226 (14)
C25	0.5104 (7)	0.5355 (7)	0.3108 (5)	0.0258 (15)
H25A	0.5077	0.4783	0.3709	0.031*
C26	0.5155 (7)	0.4933 (7)	0.2211 (5)	0.0274 (15)
H26A	0.5150	0.4068	0.2225	0.033*
C27	0.5258 (8)	0.6949 (7)	0.1321 (5)	0.0300 (16)
H27A	0.5354	0.7497	0.0703	0.036*
C28	0.5172 (7)	0.7460 (7)	0.2184 (5)	0.0262 (15)
H28A	0.5167	0.8330	0.2151	0.031*
N1	-0.1457 (5)	0.5694 (5)	0.4954 (4)	0.0197 (11)
H1	-0.1199	0.6463	0.4819	0.024*
N2	-0.1400 (7)	0.7376 (7)	0.1191 (5)	0.0352 (15)
N3	0.4213 (5)	0.8043 (5)	0.4280 (4)	0.0199 (12)
H3	0.3831	0.8460	0.3806	0.024*
N4	0.5212 (6)	0.5710 (6)	0.1323 (4)	0.0243 (13)
O1	-0.3059 (5)	0.5656 (5)	0.9346 (3)	0.0292 (11)
O2	-0.1793 (5)	0.7147 (4)	0.8335 (4)	0.0280 (11)
O3	-0.1703 (6)	0.1271 (4)	0.8379 (3)	0.0325 (12)
O4	-0.2075 (6)	0.1200 (5)	0.6898 (4)	0.0331 (12)
O5	-0.1926 (8)	0.4070 (5)	0.4251 (4)	0.0521 (18)
O6	0.0561 (5)	0.9015 (5)	0.8108 (4)	0.0279 (12)
O7	0.0016 (5)	0.9159 (6)	0.6644 (3)	0.0356 (13)
O8	0.5758 (5)	0.9079 (5)	0.8090 (4)	0.0285 (12)
O9	0.7095 (4)	0.8844 (4)	0.6686 (3)	0.0214 (10)
O10	0.5752 (5)	0.6497 (6)	0.4668 (4)	0.0357 (13)
O1W	-0.4267 (6)	0.3145 (5)	1.0665 (4)	0.0339 (12)
H1WB	-0.3591	0.2868	1.0285	0.041*
H1WA	-0.4880	0.2603	1.0843	0.041*
O2W	-0.2229 (6)	0.9033 (5)	0.9693 (4)	0.0335 (12)
H2WB	-0.1908	0.9650	0.9863	0.040*
H2WC	-0.1880	0.8351	0.9967	0.040*
O3W	0.9154 (8)	0.8418 (6)	0.4834 (4)	0.0568 (19)

H3WA	0.9711	0.8601	0.5171	0.068*
H3WB	0.8369	0.8457	0.5189	0.068*
O4W	0.8025 (7)	0.1615 (8)	0.0328 (5)	0.066 (2)
H4WA	0.8294	0.1409	-0.0248	0.079*
H4WB	0.8595	0.1331	0.0702	0.079*

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Co1	0.0270 (7)	0.0208 (7)	0.0212 (6)	-0.0031 (5)	-0.0058 (5)	-0.0071 (5)
Er1	0.0144 (2)	0.0097 (2)	0.0188 (2)	0.00035 (12)	-0.00753 (12)	-0.00390 (12)
C1	0.017 (3)	0.011 (3)	0.021 (3)	-0.001 (2)	-0.005 (2)	-0.004 (2)
C2	0.023 (3)	0.012 (3)	0.026 (3)	0.000 (3)	-0.004 (3)	-0.003 (3)
C3	0.016 (3)	0.015 (3)	0.023 (3)	0.001 (2)	-0.005 (2)	-0.003 (2)
C4	0.017 (3)	0.016 (3)	0.026 (3)	-0.002 (2)	-0.006 (3)	-0.007 (3)
C5	0.016 (3)	0.012 (3)	0.023 (3)	0.002 (2)	-0.007 (2)	-0.004 (2)
C6	0.017 (3)	0.016 (3)	0.023 (3)	-0.001 (3)	-0.007 (3)	-0.001 (3)
C7	0.014 (3)	0.018 (3)	0.021 (3)	0.000 (3)	-0.006 (2)	-0.002 (3)
C8	0.021 (3)	0.017 (3)	0.027 (3)	0.008 (3)	-0.013 (3)	-0.006 (3)
C9	0.031 (4)	0.024 (4)	0.026 (3)	0.000 (3)	-0.012 (3)	-0.005 (3)
C10	0.018 (3)	0.029 (4)	0.028 (4)	-0.001 (3)	-0.010 (3)	-0.006 (3)
C11	0.041 (4)	0.029 (4)	0.031 (4)	0.002 (3)	-0.011 (3)	-0.009 (3)
C12	0.045 (5)	0.042 (5)	0.022 (4)	0.001 (4)	-0.008 (3)	-0.011 (3)
C13	0.040 (4)	0.028 (4)	0.035 (4)	-0.007 (3)	-0.016 (3)	0.002 (3)
C14	0.032 (4)	0.030 (4)	0.026 (4)	-0.003 (3)	-0.014 (3)	-0.002 (3)
C15	0.017 (3)	0.016 (3)	0.028 (3)	0.001 (3)	-0.008 (3)	-0.006 (3)
C16	0.016 (3)	0.020 (3)	0.024 (3)	0.002 (3)	-0.012 (2)	-0.005 (3)
C17	0.022 (3)	0.014 (3)	0.022 (3)	0.000 (3)	-0.010 (3)	-0.006 (2)
C18	0.014 (3)	0.019 (3)	0.025 (3)	0.000 (2)	-0.007 (3)	-0.003 (3)
C19	0.013 (3)	0.019 (3)	0.027 (3)	-0.003 (3)	-0.008 (3)	-0.003 (3)
C20	0.022 (3)	0.023 (3)	0.019 (3)	0.002 (3)	-0.009 (3)	-0.011 (3)
C21	0.020 (3)	0.013 (3)	0.028 (3)	-0.003 (2)	-0.009 (3)	-0.006 (3)
C22	0.018 (3)	0.011 (3)	0.029 (3)	-0.006 (2)	-0.007 (3)	-0.008 (3)
C23	0.015 (3)	0.031 (4)	0.019 (3)	-0.001 (3)	-0.005 (3)	-0.006 (3)
C24	0.009 (3)	0.035 (4)	0.026 (3)	0.002 (3)	-0.003 (2)	-0.011 (3)
C25	0.031 (4)	0.030 (4)	0.020 (3)	0.002 (3)	-0.009 (3)	-0.009 (3)
C26	0.036 (4)	0.027 (4)	0.024 (3)	0.004 (3)	-0.012 (3)	-0.013 (3)
C27	0.037 (4)	0.031 (4)	0.022 (3)	-0.007 (3)	-0.006 (3)	-0.002 (3)
C28	0.026 (4)	0.029 (4)	0.028 (3)	-0.003 (3)	-0.006 (3)	-0.013 (3)
N1	0.025 (3)	0.013 (3)	0.022 (3)	0.001 (2)	-0.009 (2)	0.000 (2)
N2	0.040 (4)	0.040 (4)	0.027 (3)	-0.004 (3)	-0.016 (3)	0.001 (3)
N3	0.022 (3)	0.026 (3)	0.015 (3)	0.002 (2)	-0.010 (2)	-0.006 (2)
N4	0.021 (3)	0.029 (3)	0.026 (3)	-0.003 (2)	-0.003 (2)	-0.013 (3)
O1	0.030 (3)	0.032 (3)	0.025 (2)	-0.009 (2)	0.001 (2)	-0.009 (2)
O2	0.043 (3)	0.009 (2)	0.033 (3)	-0.005 (2)	-0.010 (2)	-0.0046 (19)
O3	0.069 (4)	0.011 (2)	0.023 (2)	-0.004 (2)	-0.020 (2)	-0.0013 (19)
O4	0.062 (4)	0.017 (3)	0.029 (3)	-0.002 (2)	-0.025 (2)	-0.007 (2)
O5	0.106 (6)	0.021 (3)	0.035 (3)	-0.020 (3)	-0.028 (3)	0.002 (2)



## supplementary materials

---

O6	0.019 (2)	0.045 (3)	0.024 (2)	-0.001 (2)	-0.0048 (19)	-0.015 (2)
O7	0.017 (2)	0.066 (4)	0.024 (2)	0.005 (2)	-0.007 (2)	-0.005 (2)
O8	0.022 (3)	0.046 (3)	0.025 (2)	-0.002 (2)	-0.009 (2)	-0.017 (2)
O9	0.012 (2)	0.026 (3)	0.029 (2)	0.0022 (18)	-0.0079 (18)	-0.010 (2)
O10	0.034 (3)	0.046 (3)	0.035 (3)	0.018 (3)	-0.021 (2)	-0.020 (2)
O1W	0.040 (3)	0.029 (3)	0.033 (3)	0.000 (2)	-0.007 (2)	-0.007 (2)
O2W	0.054 (3)	0.021 (3)	0.026 (2)	0.002 (2)	-0.016 (2)	0.000 (2)
O3W	0.104 (6)	0.038 (4)	0.032 (3)	-0.018 (4)	-0.013 (3)	-0.012 (3)
O4W	0.053 (4)	0.111 (7)	0.034 (3)	0.023 (4)	-0.015 (3)	-0.014 (4)

### Geometric parameters ( $\text{\AA}$ , $^\circ$ )

Co1—O1 <sup>i</sup>	2.095 (5)	C15—C16	1.406 (9)
Co1—O1	2.095 (5)	C15—C21	1.495 (9)
Co1—N4 <sup>ii</sup>	2.152 (5)	C16—C17	1.353 (9)
Co1—N4 <sup>iii</sup>	2.152 (5)	C16—H16A	0.9300
Co1—O1W	2.184 (5)	C17—C18	1.390 (9)
Co1—O1W <sup>i</sup>	2.184 (5)	C17—N3	1.434 (8)
Er1—O2	2.200 (5)	C18—C19	1.377 (9)
Er1—O2W	2.303 (5)	C18—H18A	0.9300
Er1—O7	2.330 (5)	C19—C20	1.389 (9)
Er1—O9 <sup>iv</sup>	2.348 (4)	C19—C22	1.498 (9)
Er1—O4 <sup>v</sup>	2.379 (5)	C20—H20A	0.9300
Er1—O3 <sup>v</sup>	2.398 (5)	C21—O7	1.245 (8)
Er1—O8 <sup>iv</sup>	2.429 (5)	C21—O6	1.266 (8)
Er1—O6	2.438 (5)	C22—O9	1.243 (8)
C1—C6	1.385 (9)	C22—O8	1.277 (8)
C1—C2	1.390 (9)	C23—O10	1.207 (8)
C1—C8	1.500 (8)	C23—N3	1.342 (9)
C2—C3	1.402 (9)	C23—C24	1.521 (9)
C2—H2A	0.9300	C24—C25	1.379 (10)
C3—C4	1.398 (9)	C24—C28	1.389 (10)
C3—N1	1.393 (8)	C25—C26	1.382 (9)
C4—C5	1.368 (9)	C25—H25A	0.9300
C4—H4A	0.9300	C26—N4	1.336 (10)
C5—C6	1.392 (9)	C26—H26A	0.9300
C5—C7	1.492 (9)	C27—N4	1.339 (10)
C6—H6A	0.9300	C27—C28	1.384 (10)
C7—O4	1.244 (8)	C27—H27A	0.9300
C7—O3	1.261 (8)	C28—H28A	0.9300
C8—O1	1.247 (8)	N1—H1	0.8600
C8—O2	1.263 (8)	N3—H3	0.8600
C9—O5	1.214 (9)	N4—Co1 <sup>vi</sup>	2.152 (5)
C9—N1	1.358 (8)	O3—Er1 <sup>vii</sup>	2.398 (5)
C9—C10	1.509 (10)	O4—Er1 <sup>vii</sup>	2.379 (5)
C10—C14	1.371 (11)	O8—Er1 <sup>viii</sup>	2.429 (5)

C10—C11	1.391 (10)	O9—Er1 <sup>viii</sup>	2.348 (4)
C11—C12	1.362 (11)	O1W—H1WB	0.8488
C11—H11A	0.9300	O1W—H1WA	0.8469
C12—N2	1.334 (11)	O2W—H2WB	0.8474
C12—H12A	0.9300	O2W—H2WC	0.8489
C13—N2	1.349 (10)	O3W—H3WA	0.8477
C13—C14	1.370 (10)	O3W—H3WB	0.8482
C13—H13A	0.9300	O4W—H4WA	0.8494
C14—H14A	0.9300	O4W—H4WB	0.8487
C15—C20	1.387 (9)		
O1 <sup>i</sup> —Co1—O1	180.0	O5—C9—C10	118.5 (6)
O1 <sup>i</sup> —Co1—N4 <sup>ii</sup>	87.4 (2)	N1—C9—C10	117.9 (6)
O1—Co1—N4 <sup>ii</sup>	92.6 (2)	C14—C10—C11	117.6 (7)
O1 <sup>i</sup> —Co1—N4 <sup>iii</sup>	92.6 (2)	C14—C10—C9	125.2 (6)
O1—Co1—N4 <sup>iii</sup>	87.4 (2)	C11—C10—C9	117.1 (7)
N4 <sup>ii</sup> —Co1—N4 <sup>iii</sup>	180.000 (1)	C12—C11—C10	119.3 (7)
O1 <sup>i</sup> —Co1—O1W	85.9 (2)	C12—C11—H11A	120.4
O1—Co1—O1W	94.1 (2)	C10—C11—H11A	120.4
N4 <sup>ii</sup> —Co1—O1W	90.5 (2)	N2—C12—C11	124.2 (7)
N4 <sup>iii</sup> —Co1—O1W	89.5 (2)	N2—C12—H12A	117.9
O1 <sup>i</sup> —Co1—O1W <sup>i</sup>	94.1 (2)	C11—C12—H12A	117.9
O1—Co1—O1W <sup>i</sup>	85.9 (2)	N2—C13—C14	123.9 (7)
N4 <sup>ii</sup> —Co1—O1W <sup>i</sup>	89.5 (2)	N2—C13—H13A	118.1
N4 <sup>iii</sup> —Co1—O1W <sup>i</sup>	90.5 (2)	C14—C13—H13A	118.1
O1W—Co1—O1W <sup>i</sup>	180.000 (1)	C13—C14—C10	119.3 (7)
O2—Er1—O2W	82.38 (18)	C13—C14—H14A	120.3
O2—Er1—O7	90.7 (2)	C10—C14—H14A	120.3
O2W—Er1—O7	138.81 (18)	C20—C15—C16	119.5 (6)
O2—Er1—O9 <sup>iv</sup>	81.92 (18)	C20—C15—C21	122.5 (6)
O2W—Er1—O9 <sup>iv</sup>	139.01 (18)	C16—C15—C21	118.0 (6)
O7—Er1—O9 <sup>iv</sup>	78.93 (16)	C17—C16—C15	120.4 (6)
O2—Er1—O4 <sup>v</sup>	153.92 (18)	C17—C16—H16A	119.8
O2W—Er1—O4 <sup>v</sup>	121.33 (17)	C15—C16—H16A	119.8
O7—Er1—O4 <sup>v</sup>	78.2 (2)	C16—C17—C18	120.4 (6)
O9 <sup>iv</sup> —Er1—O4 <sup>v</sup>	72.87 (16)	C16—C17—N3	119.6 (6)
O2—Er1—O3 <sup>v</sup>	152.42 (18)	C18—C17—N3	120.0 (6)
O2W—Er1—O3 <sup>v</sup>	71.32 (17)	C19—C18—C17	119.7 (6)
O7—Er1—O3 <sup>v</sup>	103.5 (2)	C19—C18—H18A	120.1
O9 <sup>iv</sup> —Er1—O3 <sup>v</sup>	123.62 (17)	C17—C18—H18A	120.1
O4 <sup>v</sup> —Er1—O3 <sup>v</sup>	53.59 (16)	C18—C19—C20	120.6 (6)
O2—Er1—O8 <sup>iv</sup>	85.79 (19)	C18—C19—C22	117.2 (6)
O2W—Er1—O8 <sup>iv</sup>	87.16 (18)	C20—C19—C22	122.2 (6)
O7—Er1—O8 <sup>iv</sup>	132.96 (16)	C19—C20—C15	119.3 (6)

## supplementary materials

---

O9 <sup>iv</sup> —Er1—O8 <sup>iv</sup>	54.11 (15)	C19—C20—H20A	120.4
O4 <sup>v</sup> —Er1—O8 <sup>iv</sup>	84.85 (19)	C15—C20—H20A	120.4
O3 <sup>v</sup> —Er1—O8 <sup>iv</sup>	100.68 (19)	O7—C21—O6	118.8 (6)
O2—Er1—O6	85.14 (19)	O7—C21—C15	119.9 (6)
O2W—Er1—O6	85.04 (18)	O6—C21—C15	121.3 (6)
O7—Er1—O6	53.86 (16)	O9—C22—O8	119.3 (6)
O9 <sup>iv</sup> —Er1—O6	130.75 (15)	O9—C22—C19	120.0 (6)
O4 <sup>v</sup> —Er1—O6	106.15 (19)	O8—C22—C19	120.8 (6)
O3 <sup>v</sup> —Er1—O6	84.49 (19)	O9—C22—Er1 <sup>viii</sup>	57.8 (3)
O8 <sup>iv</sup> —Er1—O6	168.74 (18)	O8—C22—Er1 <sup>viii</sup>	61.5 (3)
O2—Er1—C22 <sup>iv</sup>	83.91 (19)	C19—C22—Er1 <sup>viii</sup>	176.9 (4)
O2W—Er1—C22 <sup>iv</sup>	113.99 (19)	O10—C23—N3	125.3 (6)
O7—Er1—C22 <sup>iv</sup>	105.45 (18)	O10—C23—C24	118.6 (6)
O9 <sup>iv</sup> —Er1—C22 <sup>iv</sup>	26.61 (17)	N3—C23—C24	116.1 (6)
O4 <sup>v</sup> —Er1—C22 <sup>iv</sup>	76.62 (18)	C25—C24—C28	118.8 (6)
O3 <sup>v</sup> —Er1—C22 <sup>iv</sup>	113.96 (19)	C25—C24—C23	117.6 (6)
O8 <sup>iv</sup> —Er1—C22 <sup>iv</sup>	27.52 (17)	C28—C24—C23	123.5 (6)
O6—Er1—C22 <sup>iv</sup>	156.44 (18)	C26—C25—C24	119.1 (7)
O2—Er1—C7 <sup>v</sup>	179.27 (18)	C26—C25—H25A	120.4
O2W—Er1—C7 <sup>v</sup>	96.94 (18)	C24—C25—H25A	120.4
O7—Er1—C7 <sup>v</sup>	90.0 (2)	N4—C26—C25	123.0 (7)
O9 <sup>iv</sup> —Er1—C7 <sup>v</sup>	98.43 (17)	N4—C26—H26A	118.5
O4 <sup>v</sup> —Er1—C7 <sup>v</sup>	26.59 (17)	C25—C26—H26A	118.5
O3 <sup>v</sup> —Er1—C7 <sup>v</sup>	27.03 (17)	N4—C27—C28	123.8 (7)
O8 <sup>iv</sup> —Er1—C7 <sup>v</sup>	93.89 (19)	N4—C27—H27A	118.1
O6—Er1—C7 <sup>v</sup>	95.10 (19)	C28—C27—H27A	118.1
C22 <sup>iv</sup> —Er1—C7 <sup>v</sup>	96.11 (18)	C24—C28—C27	118.0 (7)
C6—C1—C2	120.6 (6)	C24—C28—H28A	121.0
C6—C1—C8	119.0 (6)	C27—C28—H28A	121.0
C2—C1—C8	120.3 (6)	C9—N1—C3	125.4 (6)
C1—C2—C3	120.3 (6)	C9—N1—H1	117.3
C1—C2—H2A	119.9	C3—N1—H1	117.3
C3—C2—H2A	119.9	C12—N2—C13	115.7 (6)
C4—C3—N1	122.8 (6)	C23—N3—C17	120.5 (5)
C4—C3—C2	118.7 (6)	C23—N3—H3	119.7
N1—C3—C2	118.4 (6)	C17—N3—H3	119.7
C5—C4—C3	120.0 (6)	C26—N4—C27	117.2 (6)
C5—C4—H4A	120.0	C26—N4—Co1 <sup>vi</sup>	120.6 (5)
C3—C4—H4A	120.0	C27—N4—Co1 <sup>vi</sup>	121.8 (5)
C4—C5—C6	121.9 (6)	C8—O1—Co1	143.4 (4)
C4—C5—C7	117.8 (6)	C8—O2—Er1	154.6 (5)
C6—C5—C7	120.3 (6)	C7—O3—Er1 <sup>vii</sup>	93.2 (4)
C1—C6—C5	118.4 (6)	C7—O4—Er1 <sup>vii</sup>	94.6 (4)

C1—C6—H6A	120.8	C21—O6—Er1	90.8 (4)
C5—C6—H6A	120.8	C21—O7—Er1	96.5 (4)
O4—C7—O3	118.6 (6)	C22—O8—Er1 <sup>viii</sup>	90.9 (4)
O4—C7—C5	120.5 (6)	C22—O9—Er1 <sup>viii</sup>	95.6 (4)
O3—C7—C5	120.9 (6)	Co1—O1W—H1WB	112.7
O4—C7—Er1 <sup>vii</sup>	58.9 (3)	Co1—O1W—H1WA	112.9
O3—C7—Er1 <sup>vii</sup>	59.8 (3)	H1WB—O1W—H1WA	110.2
C5—C7—Er1 <sup>vii</sup>	177.4 (5)	Er1—O2W—H2WB	110.5
O1—C8—O2	123.2 (6)	Er1—O2W—H2WC	111.1
O1—C8—C1	119.2 (6)	H2WB—O2W—H2WC	109.0
O2—C8—C1	117.6 (6)	H3WA—O3W—H3WB	107.4
O5—C9—N1	123.6 (6)	H4WA—O4W—H4WB	108.9
C6—C1—C2—C3	3.3 (10)	O5—C9—N1—C3	-5.1 (12)
C8—C1—C2—C3	-172.9 (6)	C10—C9—N1—C3	175.4 (6)
C1—C2—C3—C4	-4.1 (9)	C4—C3—N1—C9	19.7 (10)
C1—C2—C3—N1	177.7 (6)	C2—C3—N1—C9	-162.1 (6)
N1—C3—C4—C5	179.7 (6)	C11—C12—N2—C13	0.9 (12)
C2—C3—C4—C5	1.6 (9)	C14—C13—N2—C12	-1.2 (12)
C3—C4—C5—C6	1.8 (10)	O10—C23—N3—C17	-8.0 (11)
C3—C4—C5—C7	178.8 (6)	C24—C23—N3—C17	170.3 (6)
C2—C1—C6—C5	0.0 (9)	C16—C17—N3—C23	-131.1 (7)
C8—C1—C6—C5	176.2 (6)	C18—C17—N3—C23	47.8 (9)
C4—C5—C6—C1	-2.6 (10)	C25—C26—N4—C27	1.9 (11)
C7—C5—C6—C1	-179.5 (6)	C25—C26—N4—Co1 <sup>vi</sup>	-171.1 (6)
C4—C5—C7—O4	-17.8 (9)	C28—C27—N4—C26	-3.9 (11)
C6—C5—C7—O4	159.2 (6)	C28—C27—N4—Co1 <sup>vi</sup>	169.1 (6)
C4—C5—C7—O3	162.8 (6)	O2—C8—O1—Co1	120.6 (7)
C6—C5—C7—O3	-20.2 (10)	C1—C8—O1—Co1	-60.1 (10)
C6—C1—C8—O1	-26.8 (9)	N4 <sup>ii</sup> —Co1—O1—C8	29.9 (8)
C2—C1—C8—O1	149.4 (6)	N4 <sup>iii</sup> —Co1—O1—C8	-150.1 (8)
C6—C1—C8—O2	152.5 (6)	O1W—Co1—O1—C8	120.6 (8)
C2—C1—C8—O2	-31.2 (9)	O1W <sup>i</sup> —Co1—O1—C8	-59.4 (8)
O5—C9—C10—C14	164.4 (8)	O1—C8—O2—Er1	-74.1 (13)
N1—C9—C10—C14	-16.0 (11)	C1—C8—O2—Er1	106.6 (10)
O5—C9—C10—C11	-12.4 (11)	O2W—Er1—O2—C8	91.1 (11)
N1—C9—C10—C11	167.2 (6)	O7—Er1—O2—C8	-129.7 (11)
C14—C10—C11—C12	-1.0 (11)	O9 <sup>iv</sup> —Er1—O2—C8	-51.0 (11)
C9—C10—C11—C12	176.0 (7)	O4 <sup>v</sup> —Er1—O2—C8	-65.8 (12)
C10—C11—C12—N2	0.2 (13)	O3 <sup>v</sup> —Er1—O2—C8	108.5 (11)
N2—C13—C14—C10	0.4 (12)	O8 <sup>iv</sup> —Er1—O2—C8	3.4 (11)
C11—C10—C14—C13	0.7 (11)	O6—Er1—O2—C8	176.7 (11)
C9—C10—C14—C13	-176.0 (7)	C22 <sup>iv</sup> —Er1—O2—C8	-24.2 (11)
C20—C15—C16—C17	0.6 (10)	O4—C7—O3—Er1 <sup>vii</sup>	3.6 (7)
C21—C15—C16—C17	-177.6 (6)	C5—C7—O3—Er1 <sup>vii</sup>	-177.1 (5)
C15—C16—C17—C18	-2.1 (10)	O3—C7—O4—Er1 <sup>vii</sup>	-3.6 (7)

## supplementary materials

C15—C16—C17—N3	176.8 (6)	C5—C7—O4—Er1 <sup>vii</sup>	177.0 (5)
C16—C17—C18—C19	2.3 (10)	O7—C21—O6—Er1	2.5 (7)
N3—C17—C18—C19	-176.6 (6)	C15—C21—O6—Er1	-178.0 (6)
C17—C18—C19—C20	-1.0 (10)	O2—Er1—O6—C21	92.9 (4)
C17—C18—C19—C22	179.9 (6)	O2W—Er1—O6—C21	175.7 (4)
C18—C19—C20—C15	-0.5 (10)	O7—Er1—O6—C21	-1.5 (4)
C22—C19—C20—C15	178.6 (6)	O9 <sup>iv</sup> —Er1—O6—C21	17.9 (5)
C16—C15—C20—C19	0.7 (10)	O4 <sup>v</sup> —Er1—O6—C21	-63.1 (4)
C21—C15—C20—C19	178.8 (6)	O3 <sup>v</sup> —Er1—O6—C21	-112.7 (4)
C20—C15—C21—O7	166.6 (6)	O8 <sup>iv</sup> —Er1—O6—C21	129.4 (7)
C16—C15—C21—O7	-15.3 (10)	C22 <sup>iv</sup> —Er1—O6—C21	30.4 (7)
C20—C15—C21—O6	-12.9 (10)	C7 <sup>v</sup> —Er1—O6—C21	-87.8 (4)
C16—C15—C21—O6	165.2 (6)	O6—C21—O7—Er1	-2.7 (7)
C18—C19—C22—O9	4.3 (9)	C15—C21—O7—Er1	177.8 (5)
C20—C19—C22—O9	-174.8 (6)	O2—Er1—O7—C21	-82.0 (4)
C18—C19—C22—O8	-174.9 (6)	O2W—Er1—O7—C21	-2.8 (6)
C20—C19—C22—O8	6.0 (10)	O9 <sup>iv</sup> —Er1—O7—C21	-163.6 (5)
O10—C23—C24—C25	41.6 (9)	O4 <sup>v</sup> —Er1—O7—C21	121.8 (4)
N3—C23—C24—C25	-136.8 (7)	O3 <sup>v</sup> —Er1—O7—C21	74.1 (4)
O10—C23—C24—C28	-135.7 (7)	O8 <sup>iv</sup> —Er1—O7—C21	-166.9 (4)
N3—C23—C24—C28	45.9 (9)	O6—Er1—O7—C21	1.5 (4)
C28—C24—C25—C26	-1.7 (10)	C22 <sup>iv</sup> —Er1—O7—C21	-165.9 (4)
C23—C24—C25—C26	-179.1 (6)	C7 <sup>v</sup> —Er1—O7—C21	97.8 (4)
C24—C25—C26—N4	0.8 (11)	O9—C22—O8—Er1 <sup>viii</sup>	3.2 (6)
C25—C24—C28—C27	-0.1 (10)	C19—C22—O8—Er1 <sup>viii</sup>	-177.6 (5)
C23—C24—C28—C27	177.2 (6)	O8—C22—O9—Er1 <sup>viii</sup>	-3.3 (7)
N4—C27—C28—C24	3.0 (11)	C19—C22—O9—Er1 <sup>viii</sup>	177.4 (5)

Symmetry codes: (i)  $-x-1, -y+1, -z+2$ ; (ii)  $-x, -y+1, -z+1$ ; (iii)  $x-1, y, z+1$ ; (iv)  $x-1, y, z$ ; (v)  $x, y+1, z$ ; (vi)  $x+1, y, z-1$ ; (vii)  $x, y-1, z$ ; (viii)  $x+1, y, z$ .

### Hydrogen-bond geometry ( $\text{\AA}, ^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1 $\cdots$ O3W <sup>iv</sup>	0.86	2.16	3.007 (8)	166.
O1W—H1WB $\cdots$ O4W <sup>iii</sup>	0.85	2.05	2.769 (9)	142.
O1W—H1WA $\cdots$ O8 <sup>ix</sup>	0.85	2.22	2.975 (8)	149.
O2W—H2WB $\cdots$ O4W <sup>x</sup>	0.85	2.32	3.109 (10)	156.
O2W—H2WC $\cdots$ N2 <sup>xi</sup>	0.85	1.94	2.687 (8)	147.
O3W—H3WA $\cdots$ O7 <sup>viii</sup>	0.85	2.30	3.041 (8)	147.
O3W—H3WB $\cdots$ O9	0.85	2.30	3.042 (8)	147.
O4W—H4WA $\cdots$ O3 <sup>vi</sup>	0.85	1.92	2.729 (8)	159.
O4W—H4WB $\cdots$ O6 <sup>xii</sup>	0.85	1.95	2.762 (8)	159.

Symmetry codes: (iv)  $x-1, y, z$ ; (iii)  $x-1, y, z+1$ ; (ix)  $-x, -y+1, -z+2$ ; (x)  $x-1, y+1, z+1$ ; (xi)  $x, y, z+1$ ; (viii)  $x+1, y, z$ ; (vi)  $x+1, y, z-1$ ; (xii)  $-x+1, -y+1, -z+1$ .

Fig. 1

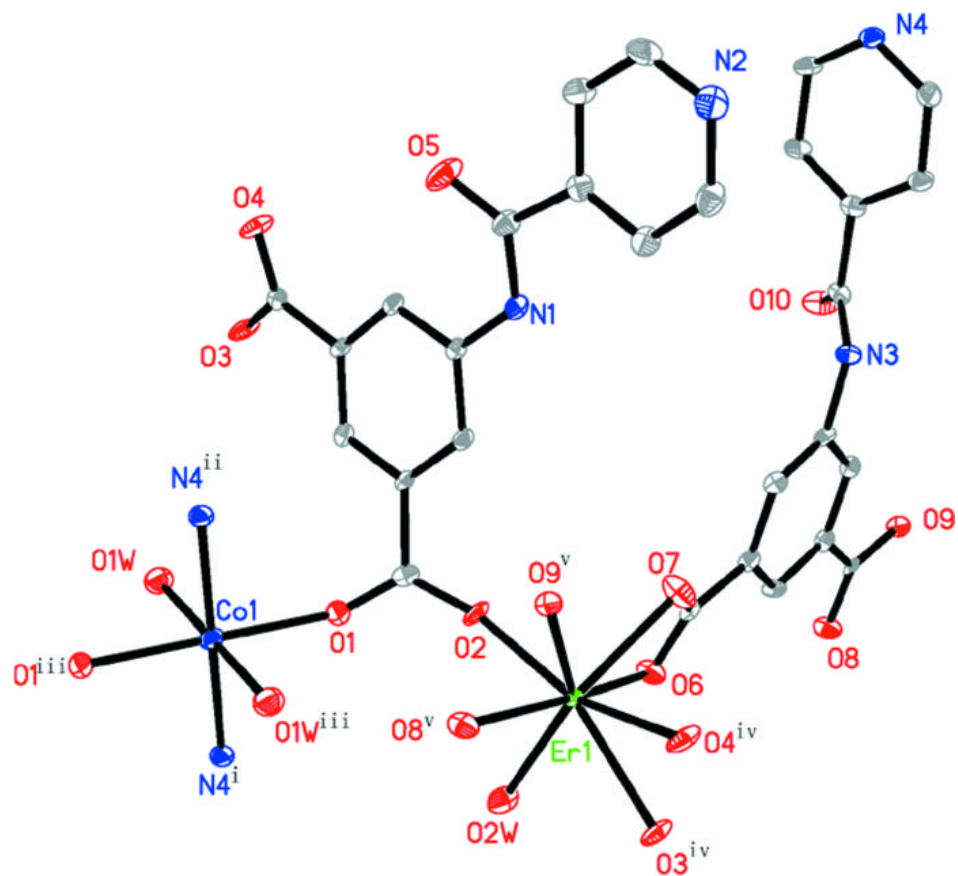


Fig. 2

