Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Diaquabis(1-naphthaleneacetato-κO)-bis(1,10-phenanthroline-$\kappa^2 N,N'$)-erbium(III) 1-naphthaleneacetate monohydrate

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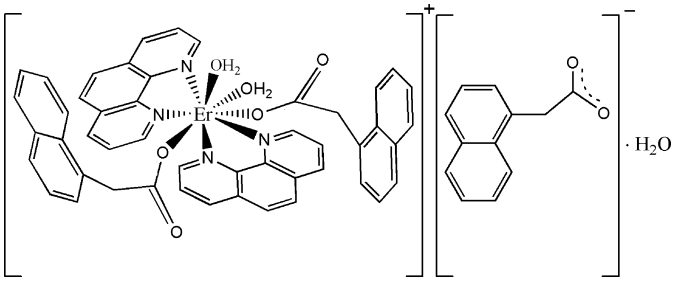
Received 11 September 2007; accepted 12 September 2007

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.031 Å; disorder in solvent or counterion; R factor = 0.078; wR factor = 0.220; data-to-parameter ratio = 13.1.

In title compound, $[Er(C_{12}H_9O_2)_2(C_{12}H_8N_2)_2(H_2O)_2]$-$(C_{12}H_9O_2)\cdot H_2O$, the carboxyl groups have only a monodentate coordination mode. The Er^{III} atom is eight-coordinated in a distorted dodecahedral environment by four O and four N atoms from two 1-naphthaleneacetic acid (NAA) ligands, two aqua ligands and two 1,10-phenanthroline (phen) ligands. A twofold rotation axis passes through Er. The molecules are linked into sheets by O—H···O and C—H···O hydrogen bonds. There is disorder in the anion and in the solvent water molecule; the site occupancies were set equal to 0.5.

Related literature

For related literature, see: An *et al.* (2005); Gawryszewska *et al.* (2005); Xu & Yan (2007).



Experimental

Crystal data

$[Er(C_{12}H_9O_2)_2(C_{12}H_8N_2)_2(H_2O)_2]$-$(C_{12}H_9O_2)\cdot H_2O$
M_r = 1137.29
Monoclinic, $C2/c$
a = 24.645 (3) Å
b = 14.1144 (19) Å
c = 18.162 (2) Å
β = 120.575 (2)°
V = 5439.4 (12) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.60 mm^{-1}
T = 298 (2) K
0.31 × 0.12 × 0.10 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.636, T_{max} = 0.856
13646 measured reflections
4691 independent reflections
3523 reflections with $I > 2\sigma(I)$
R_{int} = 0.089

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.078
$wR(F^2)$ = 0.220
S = 1.00
4691 reflections
357 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 2.52 e Å^{-3}
$\Delta\rho_{min}$ = −2.37 e Å^{-3}

Table 1
Selected bond lengths (Å).

Er1—O1	2.294 (7)	Er1—N2	2.537 (8)
Er1—O3	2.307 (7)	Er1—N1	2.561 (8)

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

D—H···A	D—H	H···A	D···A	D—H···A
C22—H22···O1	0.93	2.54	2.993 (12)	110
C6—H6···O6^{i}	0.93	2.45	3.37 (4)	171
O6—H6B···O4^{ii}	0.85	2.24	2.88 (4)	132
O6—H6A···O5	0.85	2.02	2.62 (4)	127
O3—H3B···O5^{ii}	0.85	1.87	2.52 (2)	132
O3—H3B···O4^{ii}	0.85	2.44	3.27 (2)	164
O3—H3B···O4	0.85	1.93	2.73 (2)	158
O3—H3A···O2^{ii}	0.85	1.98	2.691 (13)	140

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

The authors acknowledge the financial support of the Huaihai Institute of Technology Science Foundation.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2395).

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  doi:10.1107/S1600536807044546

supplementary materials

Acta Cryst. (2007). E**63**, m2544 [**doi:10.1107/S1600536807044546**]

Diaquabis(1-naphthaleneacetato-κO)bis(1,10-phenanthroline-$\kappa^2 N,N'$)erbium(III) 1-naphthaleneacetate monohydrate

Y.-F. Liu, H.-T. Xia, D.-Q. Wang, S.-P. Yang and Y.-L. Meng

Comment

Rare earth aromatic carboxylate complexes have received significant attention in recent years because of their special electronic structures, various coordination modes and as treasure-house of new material (An *et al.*, 2005; Xu & Yan, 2007). It is therefore of significance to investigate the crystal structures of rare earth complexes which will provide a help for understanding the optical, magnetic properties and biological activity of complexes (Gawryszewska *et al.*, 2005). As a part of our investigation of the crystal structures of rare earth NAA complexes with phen, this paper reports the syntheses and crystal structure of the a new complex, (I).

In the title complex, the erbium(III) center is eight-coordinated by four N atoms from two phen ligands and four O atoms from two NAA and two water ligands (Fig. 1). The Er atom situates at a distorted dodecahedron geometry. The Er—O distances are 2.947 (7) Å (carboxyl) and 2.307 (7) Å (water). The molecules of (I) are linked into sheets by O—H···O and C—H···O hydrogen bonds (Table 2). There are on direction-specific interactions between adjacent sheets in the three-dimensional network structure.

Experimental

To a stirred solution of 1-naphthylacetic acid (0.5586 g, 3 mmol) and 1,10-phenanthroline monohydrate (0.198 g, 1 mmol) in 30 ml me thanol, and a solution of $Er(NO_3)_3{\cdot}6H_2O$ (0.461 g, 1 mmol) in water (10 ml) was added. The mixed solution was heated to 333 K and stirred for 3 h, and then cooled to room temperature. The precipitate was washed with water and then dissolved in DMF. A colourless crystal suitable for X-ray diffraction was obtained by evaporation of DMF solution.

Refinement

All H atoms were located in a difference Fourier map and then treated as riding atoms, with C—H = distances of 0.93 (aryl), 0.97 Å (methylene), and O—H distances of 0.85, and with U_{iso}(H) = 1.2U_{eq}(C) (aryl and methylene) or 1.5U_{eq}(O) (water). The carboxylate radical methylene and H atoms bonded to C27, C27(B) and uncoordinated water were found to be disordered. The coordinates of the carboxylate radical methylene, H atom and the water were refined with the occupancies to half unity.

Figures

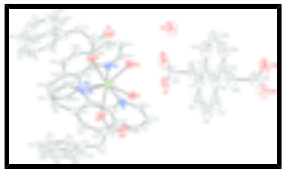


Fig. 1. The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are at the 30% probability level. For clarity, H atoms have been omitted. [Symmetry codes: (A) $1-x, y, 3/2-z$, (B) $1-x, 2-y, 2-z$].

Diaquabis(1-naphthaleneacetato-κ*O*)bis(1,10-phenanthroline- κ^2N,N')erbium(III) 1-naphthaleneacetate monohydrate

Crystal data

$[Er(C_{12}H_9O_2)_2(C_{12}H_8N_2)_2(H_2O)_2](C_{12}H_9O_2)\cdot H_2O$	$F_{000} = 2308$
$M_r = 1137.29$	$D_x = 1.389$ Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 4270 reflections
a = 24.645 (3) Å	θ = 2.4–25.1º
b = 14.1144 (19) Å	μ = 1.60 mm^{-1}
c = 18.162 (2) Å	*T* = 298 (2) K
β = 120.575 (2)º	Block, colourless
V = 5439.4 (12) Å^3	0.31 × 0.12 × 0.10 mm
Z = 4	

Data collection

Siemens SMART 1000 CCD area-detector diffractometer	4691 independent reflections
Radiation source: fine-focus sealed tube	3523 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.089$
T = 298(2) K	$\theta_{max} = 25.0$º
φ and ω scans	$\theta_{min} = 1.7$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −28→29
$T_{min} = 0.636$, $T_{max} = 0.856$	*k* = −16→15
13646 measured reflections	*l* = −21→21

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.078$	H-atom parameters constrained
$wR(F^2) = 0.220$	$w = 1/[\sigma^2(F_o^2) + (0.1579P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.00	$(\Delta/\sigma)_{max} = 0.001$
4691 reflections	$\Delta\rho_{max} = 2.52$ e Å^{-3}
357 parameters	$\Delta\rho_{min} = -2.37$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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}	Occ. (<1)
Er1	0.5000	0.53049 (3)	0.7500	0.0479 (3)	
N1	0.5510 (4)	0.5715 (6)	0.9090 (5)	0.0572 (19)	
N2	0.4950 (4)	0.3990 (6)	0.8417 (5)	0.0599 (19)	
O1	0.3989 (3)	0.4731 (5)	0.6841 (5)	0.0689 (19)	
O2	0.3239 (4)	0.5813 (9)	0.6529 (7)	0.110 (3)	
O3	0.5604 (4)	0.6579 (5)	0.7551 (4)	0.0643 (17)	
H3A	0.5976	0.6569	0.7983	0.077*	
H3B	0.5430	0.7113	0.7507	0.077*	
O4	0.5331 (13)	0.8380 (12)	0.7814 (18)	0.115 (8)	0.50
O5	0.4485 (16)	0.8284 (16)	0.7910 (18)	0.126 (8)	0.50
O6	0.3437 (15)	0.9071 (17)	0.6725 (19)	0.146 (9)	0.50
H6A	0.3616	0.8869	0.7237	0.175*	0.50
H6B	0.3699	0.9009	0.6555	0.175*	0.50
C1	0.3427 (6)	0.5022 (12)	0.6397 (8)	0.080 (3)	
C2	0.2962 (6)	0.4362 (12)	0.5690 (9)	0.091 (4)	
H2A	0.2538	0.4535	0.5544	0.109*	
H2B	0.2995	0.4458	0.5186	0.109*	
C3	0.3062 (7)	0.3329 (13)	0.5923 (10)	0.100 (5)	
C4	0.3382 (7)	0.2802 (14)	0.5617 (11)	0.110 (5)	
H4	0.3513	0.3088	0.5271	0.132*	
C5	0.3508 (8)	0.1849 (17)	0.5827 (13)	0.125 (6)	
H5	0.3722	0.1497	0.5622	0.150*	
C6	0.3313 (11)	0.1423 (18)	0.6344 (15)	0.142 (8)	
H6	0.3397	0.0785	0.6484	0.170*	
C7	0.2993 (10)	0.195 (2)	0.6651 (14)	0.131 (7)	
C8	0.2867 (7)	0.2903 (16)	0.6440 (10)	0.108 (5)	
C9	0.2547 (8)	0.3430 (16)	0.6747 (11)	0.117 (6)	
H9	0.2463	0.4068	0.6606	0.140*	
C10	0.2352 (10)	0.300 (2)	0.7263 (14)	0.145 (8)	
H10	0.2138	0.3355	0.7469	0.174*	
C11	0.2478 (10)	0.205 (2)	0.7473 (14)	0.143 (8)	
H11	0.2347	0.1764	0.7819	0.172*	
C12	0.2798 (11)	0.152 (2)	0.7167 (15)	0.147 (8)	

H12	0.2882	0.0885	0.7308	0.176*	
C13	0.5766 (6)	0.6542 (8)	0.9433 (8)	0.072 (3)	
H13	0.5691	0.7046	0.9063	0.086*	
C14	0.6140 (6)	0.6717 (9)	1.0312 (8)	0.077 (3)	
H14	0.6312	0.7313	1.0516	0.092*	
C15	0.6247 (5)	0.5977 (10)	1.0867 (7)	0.077 (3)	
H15	0.6506	0.6062	1.1454	0.093*	
C16	0.5965 (6)	0.5108 (9)	1.0544 (7)	0.066 (3)	
C17	0.5607 (5)	0.4977 (8)	0.9650 (7)	0.060 (2)	
C18	0.5315 (5)	0.4073 (8)	0.9300 (6)	0.058 (2)	
C19	0.5390 (5)	0.3316 (8)	0.9847 (7)	0.069 (3)	
C20	0.5084 (6)	0.2451 (8)	0.9483 (9)	0.079 (3)	
H20	0.5125	0.1937	0.9827	0.095*	
C21	0.4726 (6)	0.2385 (8)	0.8615 (9)	0.079 (3)	
H21	0.4520	0.1822	0.8359	0.095*	
C22	0.4671 (5)	0.3182 (7)	0.8106 (7)	0.062 (2)	
H22	0.4421	0.3124	0.7515	0.075*	
C23	0.6053 (6)	0.4298 (10)	1.1102 (8)	0.077 (3)	
H23	0.6304	0.4365	1.1692	0.092*	
C24	0.5780 (6)	0.3474 (10)	1.0772 (8)	0.080 (3)	
H24	0.5837	0.2977	1.1141	0.096*	
C25	0.492 (3)	0.872 (2)	0.794 (3)	0.122 (13)	0.50
C26	0.503 (3)	0.9720 (18)	0.826 (3)	0.125 (14)	0.50
H26A	0.5347	1.0018	0.8177	0.150*	0.50
H26B	0.4639	1.0078	0.7938	0.150*	0.50
C27	0.5229 (18)	0.9724 (12)	0.9185 (19)	0.144 (9)	
H27	0.5034	0.9691	0.8592	0.172*	0.50
C28	0.5870 (19)	0.9554 (14)	0.969 (2)	0.155 (10)	
H28	0.6098	0.9361	0.9434	0.186*	
C29	0.6169 (18)	0.9667 (13)	1.056 (2)	0.160 (11)	
H29	0.6601	0.9566	1.0895	0.192*	
C30	0.5817 (18)	0.9935 (16)	1.0932 (19)	0.155 (10)	
H30	0.6029	1.0043	1.1518	0.186*	
C31	0.4880 (17)	0.9944 (14)	0.9563 (16)	0.140 (9)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Er1	0.0420 (4)	0.0472 (4)	0.0390 (4)	0.000	0.0093 (3)	0.000
N1	0.051 (5)	0.063 (5)	0.048 (5)	−0.001 (4)	0.019 (4)	0.000 (4)
N2	0.056 (5)	0.059 (4)	0.055 (5)	0.003 (4)	0.022 (4)	0.005 (4)
O1	0.037 (4)	0.082 (5)	0.063 (5)	−0.008 (3)	0.008 (3)	0.002 (4)
O2	0.053 (5)	0.132 (8)	0.103 (7)	0.019 (6)	0.009 (5)	−0.032 (7)
O3	0.065 (4)	0.063 (4)	0.054 (4)	−0.010 (3)	0.023 (3)	−0.002 (3)
O4	0.17 (2)	0.059 (10)	0.12 (2)	0.009 (11)	0.070 (17)	−0.001 (11)
O5	0.19 (3)	0.082 (13)	0.13 (2)	0.014 (15)	0.10 (2)	−0.006 (13)
O6	0.19 (3)	0.108 (16)	0.15 (2)	0.019 (18)	0.09 (2)	0.007 (16)
C1	0.051 (7)	0.118 (9)	0.060 (7)	−0.017 (7)	0.020 (6)	−0.017 (7)

C2	0.052 (7)	0.134 (11)	0.066 (8)	−0.024 (7)	0.015 (6)	−0.021 (8)
C3	0.059 (8)	0.139 (13)	0.077 (9)	−0.036 (8)	0.017 (7)	−0.027 (9)
C4	0.069 (9)	0.138 (14)	0.087 (10)	−0.033 (9)	0.014 (8)	−0.018 (10)
C5	0.075 (11)	0.149 (17)	0.099 (13)	−0.032 (11)	0.007 (9)	−0.027 (12)
C6	0.090 (14)	0.151 (17)	0.104 (15)	−0.046 (13)	−0.010 (11)	−0.016 (14)
C7	0.086 (13)	0.16 (2)	0.093 (13)	−0.049 (14)	0.008 (10)	−0.012 (14)
C8	0.066 (9)	0.149 (15)	0.080 (10)	−0.046 (10)	0.016 (8)	−0.017 (10)
C9	0.077 (10)	0.160 (15)	0.090 (11)	−0.048 (11)	0.025 (9)	−0.015 (11)
C10	0.100 (14)	0.19 (2)	0.102 (14)	−0.049 (15)	0.020 (11)	−0.022 (14)
C11	0.095 (15)	0.18 (2)	0.103 (15)	−0.049 (16)	0.015 (12)	−0.007 (16)
C12	0.099 (15)	0.17 (2)	0.106 (15)	−0.047 (15)	0.004 (12)	−0.008 (15)
C13	0.067 (7)	0.077 (7)	0.063 (7)	−0.011 (6)	0.028 (6)	−0.007 (5)
C14	0.060 (7)	0.096 (8)	0.059 (7)	−0.015 (6)	0.019 (6)	−0.015 (6)
C15	0.055 (7)	0.108 (9)	0.050 (6)	−0.001 (6)	0.013 (5)	−0.012 (7)
C16	0.053 (6)	0.095 (7)	0.048 (6)	0.006 (5)	0.023 (5)	0.005 (5)
C17	0.051 (6)	0.077 (6)	0.054 (6)	0.004 (5)	0.029 (5)	0.003 (5)
C18	0.046 (5)	0.071 (6)	0.058 (6)	0.006 (5)	0.029 (5)	0.007 (5)
C19	0.061 (7)	0.077 (7)	0.062 (7)	0.013 (5)	0.025 (5)	0.013 (5)
C20	0.074 (8)	0.078 (7)	0.079 (9)	0.006 (6)	0.034 (7)	0.022 (6)
C21	0.067 (8)	0.065 (6)	0.087 (9)	−0.005 (5)	0.027 (7)	0.010 (6)
C22	0.051 (6)	0.059 (5)	0.066 (7)	−0.004 (4)	0.022 (5)	0.007 (5)
C23	0.068 (8)	0.102 (9)	0.051 (6)	0.011 (7)	0.023 (6)	0.010 (6)
C24	0.068 (8)	0.098 (9)	0.065 (7)	0.013 (7)	0.027 (6)	0.023 (7)
C25	0.19 (4)	0.08 (2)	0.12 (3)	0.01 (3)	0.09 (3)	0.007 (19)
C26	0.20 (5)	0.077 (19)	0.12 (3)	0.01 (2)	0.09 (3)	0.012 (16)
C27	0.22 (3)	0.090 (12)	0.13 (2)	0.009 (14)	0.09 (2)	0.012 (11)
C28	0.21 (3)	0.096 (12)	0.15 (2)	0.013 (15)	0.09 (2)	0.011 (13)
C29	0.23 (3)	0.105 (15)	0.15 (2)	0.017 (14)	0.10 (3)	0.013 (13)
C30	0.23 (4)	0.095 (12)	0.15 (2)	0.004 (17)	0.10 (3)	0.014 (14)
C31	0.22 (3)	0.084 (10)	0.129 (19)	0.019 (15)	0.10 (2)	0.010 (12)

Geometric parameters (Å, °)

Er1—O1	2.294 (7)	C10—C11	1.39 (3)
Er1—O1^{i}	2.294 (7)	C10—H10	0.9300
Er1—O3	2.307 (7)	C11—C12	1.39 (3)
Er1—O3^{i}	2.307 (7)	C11—H11	0.9300
Er1—N2^{i}	2.537 (8)	C12—H12	0.9300
Er1—N2	2.537 (8)	C13—C14	1.401 (16)
Er1—N1	2.561 (8)	C13—H13	0.9300
Er1—N1^{i}	2.561 (8)	C14—C15	1.381 (17)
N1—C13	1.322 (14)	C14—H14	0.9300
N1—C17	1.390 (14)	C15—C16	1.385 (18)
N2—C22	1.303 (13)	C15—H15	0.9300
N2—C18	1.388 (13)	C16—C17	1.411 (16)
O1—C1	1.265 (16)	C16—C23	1.468 (18)
O2—C1	1.277 (18)	C17—C18	1.444 (16)
O3—H3A	0.8500	C18—C19	1.406 (14)

O3—H3B	0.8500	C19—C20	1.411 (17)
O4—C25	1.23 (5)	C19—C24	1.467 (18)
O4—C25^{i}	1.27 (4)	C20—C21	1.362 (18)
O4—O4^{i}	1.44 (5)	C20—H20	0.9300
O4—O5^{i}	1.60 (4)	C21—C22	1.419 (15)
O5—C25	1.22 (5)	C21—H21	0.9300
O5—O4^{i}	1.60 (4)	C22—H22	0.9300
O6—H6A	0.8499	C23—C24	1.326 (19)
O6—H6B	0.8500	C23—H23	0.9300
C1—C2	1.527 (18)	C24—H24	0.9300
C2—C3	1.50 (2)	C25—O4^{i}	1.27 (4)
C2—H2A	0.9700	C25—C26	1.50 (4)
C2—H2B	0.9700	C26—C27	1.49 (5)
C3—C4	1.39 (2)	C26—H26A	0.9700
C3—C8	1.39 (2)	C26—H26B	0.9700
C4—C5	1.39 (3)	C27—C31	1.38 (4)
C4—H4	0.9300	C27—C28	1.38 (4)
C5—C6	1.39 (3)	C27—H27	0.9300
C5—H5	0.9300	C28—C29	1.37 (4)
C6—C7	1.39 (3)	C28—H28	0.9300
C6—H6	0.9300	C29—C30	1.40 (4)
C7—C12	1.39 (3)	C29—H29	0.9300
C7—C8	1.39 (3)	C30—C31^{ii}	1.49 (4)
C8—C9	1.39 (3)	C30—H30	0.9300
C9—C10	1.39 (3)	C31—C31^{ii}	1.39 (5)
C9—H9	0.9300	C31—C30^{ii}	1.49 (4)
O1—Er1—O1^{i}	138.7 (4)	C11—C10—H10	120.0
O1—Er1—O3	143.5 (3)	C12—C11—C10	120 (3)
O1^{i}—Er1—O3	75.3 (3)	C12—C11—H11	120.0
O1—Er1—O3^{i}	75.3 (3)	C10—C11—H11	120.0
O1^{i}—Er1—O3^{i}	143.5 (3)	C11—C12—C7	120 (3)
O3—Er1—O3^{i}	77.6 (4)	C11—C12—H12	120.0
O1—Er1—N2^{i}	78.6 (3)	C7—C12—H12	120.0
O1^{i}—Er1—N2^{i}	71.5 (3)	N1—C13—C14	124.9 (11)
O3—Er1—N2^{i}	110.5 (2)	N1—C13—H13	117.6
O3^{i}—Er1—N2^{i}	142.2 (3)	C14—C13—H13	117.6
O1—Er1—N2	71.5 (3)	C15—C14—C13	118.0 (11)
O1^{i}—Er1—N2	78.6 (3)	C15—C14—H14	121.0
O3—Er1—N2	142.2 (3)	C13—C14—H14	121.0
O3^{i}—Er1—N2	110.5 (2)	C14—C15—C16	119.4 (10)
N2^{i}—Er1—N2	86.0 (4)	C14—C15—H15	120.3
O1—Er1—N1	116.6 (3)	C16—C15—H15	120.3
O1^{i}—Er1—N1	73.2 (3)	C15—C16—C17	119.3 (11)
O3—Er1—N1	80.9 (2)	C15—C16—C23	122.0 (11)

O3^{i}—Er1—N1	78.8 (3)	C17—C16—C23	118.6 (12)
N2^{i}—Er1—N1	138.2 (3)	N1—C17—C16	121.2 (10)
N2—Er1—N1	65.5 (3)	N1—C17—C18	118.6 (9)
O1—Er1—N1^{i}	73.2 (3)	C16—C17—C18	120.1 (10)
O1^{i}—Er1—N1^{i}	116.6 (3)	N2—C18—C19	121.9 (10)
O3—Er1—N1^{i}	78.8 (3)	N2—C18—C17	117.9 (9)
O3^{i}—Er1—N1^{i}	80.9 (2)	C19—C18—C17	120.2 (10)
N2^{i}—Er1—N1^{i}	65.5 (3)	C18—C19—C20	118.6 (11)
N2—Er1—N1^{i}	138.2 (3)	C18—C19—C24	117.9 (11)
N1—Er1—N1^{i}	153.9 (4)	C20—C19—C24	123.4 (11)
C13—N1—C17	117.0 (9)	C21—C20—C19	118.6 (10)
C13—N1—Er1	125.0 (7)	C21—C20—H20	120.7
C17—N1—Er1	117.3 (7)	C19—C20—H20	120.7
C22—N2—C18	117.6 (9)	C20—C21—C22	119.4 (11)
C22—N2—Er1	123.1 (7)	C20—C21—H21	120.3
C18—N2—Er1	118.5 (6)	C22—C21—H21	120.3
C1—O1—Er1	139.9 (8)	N2—C22—C21	123.8 (11)
Er1—O3—H3A	113.2	N2—C22—H22	118.1
Er1—O3—H3B	113.7	C21—C22—H22	118.1
H3A—O3—H3B	110.9	C24—C23—C16	120.6 (11)
C25—O4—C25^{i}	93 (4)	C24—C23—H23	119.7
C25—O4—O4^{i}	56 (3)	C16—C23—H23	119.7
C25^{i}—O4—O4^{i}	54 (3)	C23—C24—C19	122.4 (11)
C25—O4—O5^{i}	141 (4)	C23—C24—H24	118.8
C25^{i}—O4—O5^{i}	49 (3)	C19—C24—H24	118.8
O4^{i}—O4—O5^{i}	92 (3)	O5—C25—O4	126 (3)
C25—O5—O4^{i}	51 (2)	O5—C25—O4^{i}	80 (4)
H6A—O6—H6B	107.2	O4—C25—O4^{i}	70 (3)
O1—C1—O2	123.3 (12)	O5—C25—C26	117 (4)
O1—C1—C2	116.6 (13)	O4—C25—C26	116 (5)
O2—C1—C2	120.1 (13)	O4^{i}—C25—C26	132 (3)
C3—C2—C1	114.2 (13)	O5—C25—C25^{i}	123 (5)
C3—C2—H2A	108.7	O4—C25—C25^{i}	45 (3)
C1—C2—H2A	108.7	O4^{i}—C25—C25^{i}	43 (2)
C3—C2—H2B	108.7	C26—C25—C25^{i}	106 (2)
C1—C2—H2B	108.7	C27—C26—C25	110 (3)
H2A—C2—H2B	107.6	C27—C26—H26A	109.7
C4—C3—C8	120.0 (18)	C25—C26—H26A	109.7
C4—C3—C2	116.9 (15)	C27—C26—H26B	109.7
C8—C3—C2	123.1 (17)	C25—C26—H26B	109.7
C5—C4—C3	120.0 (18)	H26A—C26—H26B	108.2
C5—C4—H4	120.0	C31—C27—C28	120 (3)
C3—C4—H4	120.0	C31—C27—C26	129 (4)
C6—C5—C4	120 (2)	C28—C27—C26	111 (3)

C6—C5—H5	120.0	C31—C27—H27	120.0
C4—C5—H5	120.0	C28—C27—H27	120.0
C5—C6—C7	120 (2)	C26—C27—H27	10.1
C5—C6—H6	120.0	C29—C28—C27	120 (3)
C7—C6—H6	120.0	C29—C28—H28	119.8
C12—C7—C8	120 (3)	C27—C28—H28	119.8
C12—C7—C6	120 (3)	C28—C29—C30	119 (3)
C8—C7—C6	120 (2)	C28—C29—H29	120.4
C3—C8—C7	120 (2)	C30—C29—H29	120.4
C3—C8—C9	120 (2)	C29—C30—C31^{ii}	123 (3)
C7—C8—C9	120 (2)	C29—C30—H30	118.4
C10—C9—C8	120 (2)	C31^{ii}—C30—H30	118.4
C10—C9—H9	120.0	C27—C31—C31^{ii}	126 (4)
C8—C9—H9	120.0	C27—C31—C30^{ii}	123 (3)
C9—C10—C11	120 (3)	C31^{ii}—C31—C30^{ii}	111 (3)
C9—C10—H10	120.0		
O1—Er1—N1—C13	−126.0 (9)	Er1—N1—C13—C14	−168.1 (9)
O1^{i}—Er1—N1—C13	97.4 (9)	N1—C13—C14—C15	−0.9 (18)
O3—Er1—N1—C13	20.1 (9)	C13—C14—C15—C16	−2.4 (17)
O3^{i}—Er1—N1—C13	−58.9 (9)	C14—C15—C16—C17	4.2 (17)
N2^{i}—Er1—N1—C13	130.8 (8)	C14—C15—C16—C23	−179.2 (11)
N2—Er1—N1—C13	−177.8 (10)	C13—N1—C17—C16	−0.2 (14)
N1^{i}—Er1—N1—C13	−19.2 (8)	Er1—N1—C17—C16	170.8 (8)
O1—Er1—N1—C17	63.7 (7)	C13—N1—C17—C18	177.6 (9)
O1^{i}—Er1—N1—C17	−72.8 (7)	Er1—N1—C17—C18	−11.3 (11)
O3—Er1—N1—C17	−150.1 (7)	C15—C16—C17—N1	−2.9 (16)
O3^{i}—Er1—N1—C17	130.9 (7)	C23—C16—C17—N1	−179.6 (9)
N2^{i}—Er1—N1—C17	−39.4 (8)	C15—C16—C17—C18	179.3 (10)
N2—Er1—N1—C17	12.0 (6)	C23—C16—C17—C18	2.5 (15)
N1^{i}—Er1—N1—C17	170.5 (7)	C22—N2—C18—C19	0.5 (14)
O1—Er1—N2—C22	45.6 (8)	Er1—N2—C18—C19	−170.0 (7)
O1^{i}—Er1—N2—C22	−105.5 (8)	C22—N2—C18—C17	−177.8 (9)
O3—Er1—N2—C22	−152.5 (7)	Er1—N2—C18—C17	11.8 (11)
O3^{i}—Er1—N2—C22	111.4 (8)	N1—C17—C18—N2	−0.1 (13)
N2^{i}—Er1—N2—C22	−33.6 (7)	C16—C17—C18—N2	177.7 (9)
N1—Er1—N2—C22	177.9 (9)	N1—C17—C18—C19	−178.4 (9)
N1^{i}—Er1—N2—C22	11.9 (10)	C16—C17—C18—C19	−0.5 (14)
O1—Er1—N2—C18	−144.5 (7)	N2—C18—C19—C20	0.0 (15)
O1^{i}—Er1—N2—C18	64.4 (7)	C17—C18—C19—C20	178.2 (10)
O3—Er1—N2—C18	17.4 (9)	N2—C18—C19—C24	−179.3 (9)
O3^{i}—Er1—N2—C18	−78.7 (7)	C17—C18—C19—C24	−1.1 (14)
N2^{i}—Er1—N2—C18	136.3 (8)	C18—C19—C20—C21	−0.2 (17)
N1—Er1—N2—C18	−12.2 (6)	C24—C19—C20—C21	179.1 (11)
N1^{i}—Er1—N2—C18	−178.3 (6)	C19—C20—C21—C22	−0.1 (18)

O1^{i}—Er1—O1—C1	−170.1 (13)	C18—N2—C22—C21	−0.8 (15)
O3—Er1—O1—C1	−17.1 (15)	Er1—N2—C22—C21	169.1 (8)
O3^{i}—Er1—O1—C1	26.1 (12)	C20—C21—C22—N2	0.7 (18)
N2^{i}—Er1—O1—C1	−126.3 (13)	C15—C16—C23—C24	−179.6 (12)
N2—Er1—O1—C1	144.1 (13)	C17—C16—C23—C24	−3.0 (17)
N1—Er1—O1—C1	95.2 (13)	C16—C23—C24—C19	1.3 (19)
N1^{i}—Er1—O1—C1	−58.6 (12)	C18—C19—C24—C23	0.7 (17)
Er1—O1—C1—O2	−38 (2)	C20—C19—C24—C23	−178.6 (12)
Er1—O1—C1—C2	143.5 (11)	O4^{i}—O5—C25—O4	−56 (4)
O1—C1—C2—C3	37.5 (17)	O4^{i}—O5—C25—C26	132 (5)
O2—C1—C2—C3	−141.0 (15)	O4^{i}—O5—C25—C25^{i}	−2(3)
C1—C2—C3—C4	−100.0 (15)	C25^{i}—O4—C25—O5	102 (7)
C1—C2—C3—C8	78.1 (17)	O4^{i}—O4—C25—O5	61 (5)
C8—C3—C4—C5	0(2)	O5^{i}—O4—C25—O5	99 (5)
C2—C3—C4—C5	178.2 (13)	C25^{i}—O4—C25—O4^{i}	42 (3)
C3—C4—C5—C6	0(2)	O5^{i}—O4—C25—O4^{i}	39 (5)
C4—C5—C6—C7	0(2)	C25^{i}—O4—C25—C26	−86 (3)
C5—C6—C7—C12	180.0 (16)	O4^{i}—O4—C25—C26	−128 (4)
C5—C6—C7—C8	0(3)	O5^{i}—O4—C25—C26	−89 (6)
C4—C3—C8—C7	0(2)	O4^{i}—O4—C25—C25^{i}	−42 (3)
C2—C3—C8—C7	−178.1 (14)	O5^{i}—O4—C25—C25^{i}	−3(4)
C4—C3—C8—C9	180.0 (14)	O5—C25—C26—C27	67 (6)
C2—C3—C8—C9	2(2)	O4—C25—C26—C27	−105 (5)
C12—C7—C8—C3	−180.0 (14)	O4^{i}—C25—C26—C27	168 (6)
C6—C7—C8—C3	0(2)	C25^{i}—C25—C26—C27	−152 (5)
C12—C7—C8—C9	0(2)	C25—C26—C27—C31	−103 (4)
C6—C7—C8—C9	180.0 (15)	C25—C26—C27—C28	82 (4)
C3—C8—C9—C10	180.0 (14)	C31—C27—C28—C29	−5(3)
C7—C8—C9—C10	0(2)	C26—C27—C28—C29	170 (2)
C8—C9—C10—C11	0(3)	C27—C28—C29—C30	1(3)
C9—C10—C11—C12	0(3)	C28—C29—C30—C31^{ii}	3(3)
C10—C11—C12—C7	0(3)	C28—C27—C31—C31^{ii}	3(4)
C8—C7—C12—C11	0(3)	C26—C27—C31—C31^{ii}	−171 (3)
C6—C7—C12—C11	−180.0 (18)	C28—C27—C31—C30^{ii}	−175 (2)
C17—N1—C13—C14	2.2 (16)	C26—C27—C31—C30^{ii}	11 (4)

Symmetry codes: (i) −*x*+1, *y*, −*z*+3/2; (ii) −*x*+1, −*y*+2, −*z*+2.

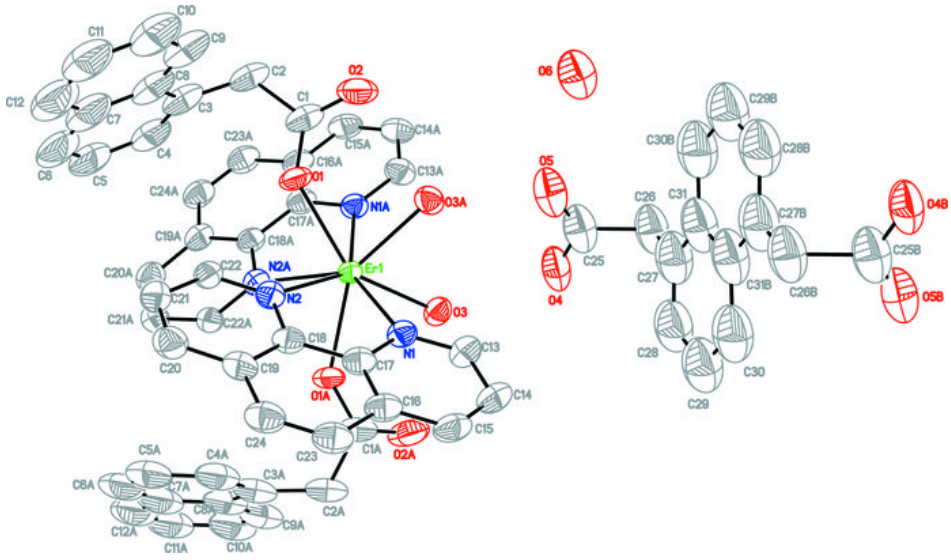
Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C22—H22···O1	0.93	2.54	2.993 (12)	110
C6—H6···O6^{iii}	0.93	2.45	3.37 (4)	171
O6—H6B···O4^{i}	0.85	2.24	2.88 (4)	132
O6—H6A···O5	0.85	2.02	2.62 (4)	127

O3—H3B···O5^{i}	0.85	1.87	2.52 (2)	132
O3—H3B···O4^{i}	0.85	2.44	3.27 (2)	164
O3—H3B···O4	0.85	1.93	2.73 (2)	158
O3—H3A···O2^{i}	0.85	1.98	2.691 (13)	140

Symmetry codes: (iii) *x*, *y*−1, *z*; (i) −*x*+1, *y*, −*z*+3/2.

Fig. 1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