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catena-Poly[diaquatris(μ_3-biphenyl-2,2′-dicarboxylato)dierbium(III)]

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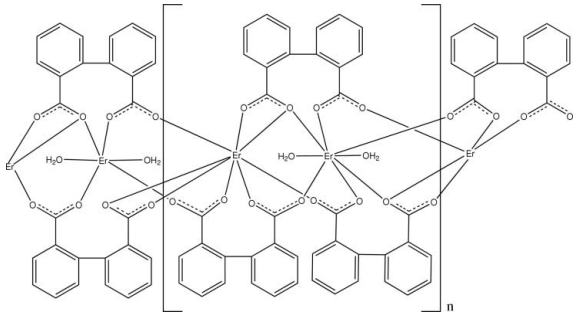
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.007 Å; R factor = 0.029; wR factor = 0.069; data-to-parameter ratio = 15.5.

The title rare earth metal coordination polymer, $[Er_2(C_{14}H_8O_4)_3(H_2O)_2]_n$, has been synthesized through a hydrothermal reaction and characterized by thermogravimetric analysis and single-crystal X-ray diffraction. The Er^{III} ions both lie on crystallographic twofold rotation axes. There are one and a half organic ligands in the asymmetric unit. Both Er ions are coordinated by eight O atoms. Whereas one is bonded only to organic ligands, the other is also coordinated by two water molecules.

Related literature

For related literature, see: Chang *et al.* (2005); Cao *et al.* (2002); Guo *et al.* (2005); Moulton & Zaworotko (2001); Ren *et al.* (2005); Rueff *et al.* (2002); Serpaggi & Ferey (1999); Serre & Ferey (2002); Thirumurugan *et al.* (2003, 2004); Wang *et al.* (2002); Zhao *et al.* (2004).



Experimental

Crystal data

$[Er_2(C_{14}H_8O_4)_3(H_2O)_2]$
M_r = 545.58
Monoclinic, $C2/c$
a = 20.9203 (19) Å
b = 21.295 (2) Å
c = 8.1553 (8) Å
β = 104.149 (1)°
V = 3522.9 (6) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 4.81 mm^{-1}
T = 298 (2) K
0.25 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.330, T_{max} = 0.424
11380 measured reflections
4076 independent reflections
3041 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.069
S = 1.00
4076 reflections
263 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.92 e Å^{-3}
$\Delta\rho_{min}$ = −0.92 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Er1—O6	2.237 (3)	Er2—O2	2.250 (3)
Er1—O4	2.409 (3)	Er2—O3	2.353 (3)
Er1—O1	2.413 (3)	Er2—O4^{i}	2.563 (3)
Er1—O5	2.424 (3)	Er2—O7^{i}	2.556 (3)
O6—Er1—O6^{ii}	87.60 (15)	O1—Er1—O1^{ii}	108.51 (14)
O6—Er1—O4^{ii}	77.96 (10)	O6—Er1—O5	147.08 (11)
O6—Er1—O4	72.81 (10)	O4—Er1—O5	139.53 (10)
O4^{ii}—Er1—O4	139.12 (14)	O6^{ii}—Er1—O5^{ii}	147.08 (11)
O6—Er1—O1	146.49 (10)	O1^{ii}—Er1—O5^{ii}	66.43 (10)
O6^{ii}—Er1—O1	90.54 (11)	O2—Er2—O7^{iii}	149.88 (11)
O4^{ii}—Er1—O1	133.02 (10)	O7^{ii}—Er2—O4^{i}	126.24 (10)
O4—Er1—O1	74.08 (10)	O3—Er2—O4^{i}	148.00 (10)
O6—Er1—O1^{ii}	90.54 (11)	O3^{i}—Er2—O4^{i}	52.62 (9)

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

Data collection: *SMART* (Bruker, 2002); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2002); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2544).

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supplementary materials

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catena-Poly[diaquatris(μ_3-biphenyl-2,2'-dicarboxylato)dierbium(III)]

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Comment

The wide spread contemporary interest in organic–inorganic hybrid material reflects their potential applications as molecular adsorption, catalysis, electromagnetism and photochemistry (Moulton & Zaworotko, 2001; Cao *et al.*, 2002). To get insight into their intriguing frameworks and properties, an enormous amount of research is being focused in using versatile organic ligands and functional metal ions to construct the novel polymers (Chang *et al.*, 2005). The role of organic carboxylic acid ligand in synthesis such materials are of great interest. In this report, we use 2,2'-biphenyldicarboxylic acid as structural directors to construct frameworks. They can compensate charges, fill space and coordinate directly to the metal center (Thirumurugan *et al.*, 2003). Recently, a series of coordination polymers of diphenic acid were reported. Most of them are based on transitional metal with diphenic acid such as $[Mn_2(2,2'\text{-dipha})_2(phen)]_n$ (Ren *et al.*, 2005) $[M_2(O_2CC_{12}H_8CO_2)_2(H_2O)_8]$ [*M* = Cobalt(II), Nickel(II)] (Rueff *et al.*, 2002), $M(bpdc)_{1.5}(H_2O)\cdot 0.5DMF$ (*M*)= Tb (1), Ho (2), Er(3), or Y (4)) (Guo *et al.*, 2005) *etc*. As the functional metal centers, rare earth metals are attracting more attention for their coordination properties and chemical characteristics (Wang *et al.*, 2002). Considering rare earth metal has high affinity for multicarboxylic acid, diphenic acid has been used as ligands for construct new frame work (Serre & Ferey, 2002; Zhao *et al.*, 2004; Serpaggi & Ferey, 1999). In this communication, hydrothermal technique has been used for their great advantages over other methods for syntheses of high-dimensional coordination compounds. We herein reported a diphenic acid compound $[Er_2(H_2O)_2(C_{14}H_8O_4)_3]_n$ (1) with one-dimensional chain employing hydrothermal method.

As illustrated in Fig. 1, in the asymmetric unit there are two crystalographically distinct Er(III) ions. The Er1 center is coordinated by eight oxygen atoms from three diphenic acid anions and two coordinated water moleculars, while the Er2 center is eight coordinated as well surrounded by eight oxygen atoms from four diphenic acid anions. The coordination geometry around them may be described as a square antiprism. The distances of Er—O bonds range from 2.237 (3) Å to 2.563 (3) Å. The O—Er—O bond angles are in the range 52.62 (9)° to 149.88 (11)°. All of them are a little bigger than those observed for other related Ln(III) complexes (Thirumurugan *et al.*, 2003, 2004). All carboxyl groups of diphenate anion ligand are deprotonated. Er ions are interconnected through $-COO^-$ groups of two diphenylcarboxylate anion ligands forming chains (Fig. 2). The phenyl rings of the ligands which are around the Er ions in adjacent chains are interdigitated and form channels in the c direction (Fig. 2)

Thermogravimetric analyses (TGA) of compound (1) were performed in air in the temperature range 35 to 500°C. It is seen from the TGA curve of $[Er_2(H_2O)_2(C_{14}H_8O_4)_3]_n$ which indicates two weight losses. The first weight loss of 3.9% around 231°C corresponds to removal of the coordinating water molecules. The second weight loss of 68.91% around 478°C is attributed to the loss of diphenate.

Experimental

The title compound was synthesized hydrothermally from $Er(NO_3)_3\cdot 6H_2O$, diphenic acid, distilled water (molar ratio: 1:1.5:10) and adding 1,3-diaminopropane until the pH value of the reaction mixture was adjusted to about 6. The resulting

mixture was stirred for about one hour at room temperature, sealed in a 25 mL Teflon tined stainless steel autoclave and heated at 170 °C for three days. After the reaction mixture was gradually cooled to room temperature, crystals suitable for single-crystal X-ray diffraction analysis were achieved.

Refinement

H atoms bonded to C were included in calculated positions, constrained to an ideal geometry with C—H = 0.93 Å and with $U_{iso}(H) = 1.2U_{eq}(C)$. The H atoms of the water molecules could not be located in a difference map and were omitted from refinement.

Figures

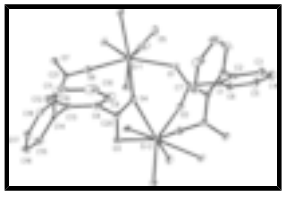

Fig. 1. Coordination environment of the Er ions in the compound (1) with thermal ellipsoid at 50% probability; all hydrogen atoms have been omitted for clarity.

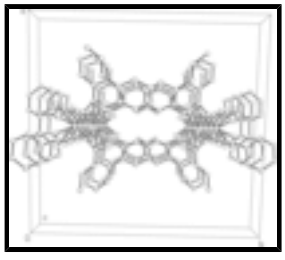

Fig. 2. Packing of compound (1) viewed along the c direction.

catena-Poly[diaquatris(μ$_3$-biphenyl-2,2'-dicarboxylato)dierbium(III)]

Crystal data

$[Er_2(C_{14}H_8O_4)_3(H_2O)_2]$	$Z = 8$
$M_r = 545.58$	$F_{000} = 2112$
Monoclinic, $C2/c$	$D_x = 2.057$ Mg m^{-3}
Hall symbol: -C 2yc	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 20.9203$ (19) Å	$\theta = 1.9$–28.3º
$b = 21.295$ (2) Å	$\mu = 4.81$ mm^{-1}
$c = 8.1553$ (8) Å	$T = 298$ (2) K
$\beta = 104.149$ (1)º	Block, pink
$V = 3522.9$ (6) Å^3	0.25 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer	4076 independent reflections
Radiation source: fine-focus sealed tube	3041 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.035$

T = 298(2) K	θ_{max} = 28.3º
φ and ω scans	θ_{min} = 1.9º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −26→21
T_{min} = 0.330, T_{max} = 0.424	k = −27→27
11380 measured reflections	l = −10→9

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.029	H-atom parameters constrained
$wR(F^2)$ = 0.069	$w = 1/[\sigma^2(F_o^2) + (0.0301P)^2 + 1.0657P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.00	$(\Delta/\sigma)_{max} < 0.001$
4076 reflections	$\Delta\rho_{max}$ = 0.92 e Å^{-3}
263 parameters	$\Delta\rho_{min}$ = −0.91 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}
Er1	0.0000	0.286068 (11)	−0.2500	0.01742 (8)
Er2	0.0000	0.207737 (11)	0.2500	0.01666 (8)
O1	0.03360 (15)	0.35226 (14)	−0.0038 (4)	0.0270 (7)
O2	0.06559 (15)	0.28775 (12)	0.2149 (4)	0.0224 (7)
O3	−0.09534 (15)	0.16647 (14)	0.0661 (4)	0.0294 (8)
O4	−0.05676 (14)	0.24656 (14)	−0.0475 (3)	0.0231 (7)
O6	−0.06811 (15)	0.21025 (12)	−0.3784 (4)	0.0237 (7)
O7	−0.04653 (16)	0.14925 (14)	−0.5796 (4)	0.0272 (7)
O5	0.08921 (17)	0.35709 (16)	−0.2627 (4)	0.0426 (10)
H5A	0.1042	0.3822	−0.1812	0.051*
H5C	0.1056	0.3568	−0.3483	0.051*
C1	0.0780 (2)	0.39592 (19)	0.2697 (5)	0.0208 (9)

C2	0.0360 (2)	0.44492 (19)	0.2913 (5)	0.0214 (10)
C3	0.0629 (2)	0.4955 (2)	0.3965 (6)	0.0311 (12)
H3A	0.0358	0.5286	0.4112	0.037*
C4	0.1290 (3)	0.4967 (2)	0.4785 (6)	0.0379 (13)
H4A	0.1461	0.5310	0.5457	0.045*
C5	0.1697 (3)	0.4476 (2)	0.4613 (6)	0.0365 (12)
H5B	0.2139	0.4481	0.5188	0.044*
C6	0.1440 (2)	0.3975 (2)	0.3575 (6)	0.0282 (11)
H6A	0.1714	0.3643	0.3463	0.034*
C7	0.0566 (2)	0.34130 (19)	0.1496 (6)	0.0194 (9)
C8	−0.1672 (2)	0.2098 (2)	−0.1767 (6)	0.0236 (10)
C9	−0.2079 (3)	0.2597 (2)	−0.1626 (6)	0.0355 (12)
H9A	−0.1921	0.2913	−0.0845	0.043*
C10	−0.2720 (3)	0.2636 (3)	−0.2632 (7)	0.0431 (14)
H10A	−0.2995	0.2966	−0.2502	0.052*
C11	−0.2937 (3)	0.2176 (3)	−0.3821 (7)	0.0406 (15)
H11A	−0.3359	0.2202	−0.4525	0.049*
C12	−0.2537 (2)	0.1673 (2)	−0.3985 (6)	0.0328 (12)
H12A	−0.2697	0.1366	−0.4792	0.039*
C13	−0.1897 (2)	0.1619 (2)	−0.2959 (5)	0.0234 (10)
C14	−0.1518 (2)	0.1043 (2)	−0.3118 (5)	0.0255 (10)
C15	−0.1762 (3)	0.0473 (2)	−0.2683 (6)	0.0381 (13)
H15A	−0.2135	0.0477	−0.2254	0.046*
C16	−0.1473 (3)	−0.0094 (2)	−0.2866 (6)	0.0430 (14)
H16A	−0.1645	−0.0464	−0.2548	0.052*
C17	−0.0926 (3)	−0.0112 (2)	−0.3524 (7)	0.0415 (14)
H17A	−0.0719	−0.0491	−0.3625	0.050*
C18	−0.0690 (3)	0.0440 (2)	−0.4027 (6)	0.0329 (12)
H18A	−0.0332	0.0426	−0.4513	0.039*
C19	−0.0969 (2)	0.1018 (2)	−0.3835 (5)	0.0218 (10)
C20	−0.1019 (2)	0.20617 (19)	−0.0487 (6)	0.0220 (10)
C21	−0.0687 (2)	0.15816 (19)	−0.4508 (5)	0.0204 (9)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Er1	0.02072 (17)	0.01736 (14)	0.01423 (15)	0.000	0.00441 (12)	0.000
Er2	0.02009 (16)	0.01609 (14)	0.01403 (15)	0.000	0.00461 (12)	0.000
O1	0.040 (2)	0.0251 (17)	0.0147 (16)	−0.0022 (14)	0.0055 (15)	0.0003 (12)
O2	0.0242 (18)	0.0203 (16)	0.0225 (17)	−0.0009 (12)	0.0056 (14)	0.0025 (12)
O3	0.0293 (19)	0.0292 (18)	0.0260 (18)	−0.0065 (14)	−0.0004 (15)	0.0065 (14)
O4	0.0234 (18)	0.0301 (17)	0.0150 (16)	−0.0055 (13)	0.0032 (14)	0.0009 (12)
O6	0.0251 (18)	0.0239 (17)	0.0243 (18)	−0.0046 (12)	0.0101 (15)	−0.0036 (12)
O7	0.041 (2)	0.0248 (16)	0.0201 (17)	−0.0063 (14)	0.0161 (16)	−0.0021 (13)
O5	0.050 (2)	0.051 (2)	0.033 (2)	−0.0262 (18)	0.0206 (18)	−0.0179 (17)
C1	0.026 (3)	0.020 (2)	0.019 (2)	−0.0024 (18)	0.010 (2)	−0.0031 (17)
C2	0.032 (3)	0.018 (2)	0.018 (2)	−0.0043 (17)	0.012 (2)	−0.0005 (16)
C3	0.037 (3)	0.023 (2)	0.040 (3)	−0.005 (2)	0.022 (3)	−0.008 (2)

C4	0.046 (4)	0.035 (3)	0.036 (3)	−0.013 (2)	0.016 (3)	−0.016 (2)
C5	0.029 (3)	0.050 (3)	0.029 (3)	−0.008 (2)	0.005 (2)	−0.013 (2)
C6	0.032 (3)	0.030 (3)	0.025 (3)	−0.001 (2)	0.012 (2)	−0.005 (2)
C7	0.016 (2)	0.018 (2)	0.028 (2)	0.0001 (17)	0.0117 (19)	0.0004 (17)
C8	0.017 (2)	0.033 (3)	0.020 (2)	−0.0025 (18)	0.005 (2)	0.0062 (18)
C9	0.037 (3)	0.045 (3)	0.028 (3)	0.007 (2)	0.016 (3)	0.006 (2)
C10	0.030 (3)	0.057 (4)	0.049 (4)	0.012 (3)	0.023 (3)	0.018 (3)
C11	0.017 (3)	0.068 (4)	0.037 (3)	−0.005 (2)	0.005 (2)	0.024 (3)
C12	0.024 (3)	0.048 (3)	0.023 (3)	−0.011 (2)	0.000 (2)	0.010 (2)
C13	0.017 (2)	0.033 (2)	0.022 (2)	−0.0061 (19)	0.0065 (19)	0.0066 (19)
C14	0.026 (3)	0.032 (3)	0.013 (2)	−0.013 (2)	−0.004 (2)	0.0005 (18)
C15	0.037 (3)	0.047 (3)	0.030 (3)	−0.017 (2)	0.006 (2)	0.008 (2)
C16	0.061 (4)	0.028 (3)	0.033 (3)	−0.017 (3)	−0.001 (3)	0.012 (2)
C17	0.058 (4)	0.024 (3)	0.037 (3)	−0.008 (3)	0.000 (3)	0.001 (2)
C18	0.046 (3)	0.029 (3)	0.021 (3)	−0.005 (2)	0.003 (2)	0.000 (2)
C19	0.023 (2)	0.027 (2)	0.014 (2)	−0.0055 (18)	0.0020 (19)	0.0021 (17)
C20	0.021 (2)	0.028 (2)	0.018 (2)	0.0008 (18)	0.007 (2)	−0.0044 (17)
C21	0.020 (2)	0.023 (2)	0.017 (2)	−0.0014 (18)	0.0013 (19)	0.0039 (17)

Geometric parameters (Å, °)

Er1—O6	2.237 (3)	C2—C2^{ii}	1.492 (9)
Er1—O6^{i}	2.237 (3)	C3—C4	1.381 (7)
Er1—O4^{i}	2.409 (3)	C3—H3A	0.9300
Er1—O4	2.409 (3)	C4—C5	1.377 (7)
Er1—O1	2.413 (3)	C4—H4A	0.9300
Er1—O1^{i}	2.413 (3)	C5—C6	1.386 (6)
Er1—O5	2.424 (3)	C5—H5B	0.9300
Er1—O5^{i}	2.424 (3)	C6—H6A	0.9300
Er2—O2	2.250 (3)	C8—C9	1.384 (6)
Er2—O2^{ii}	2.250 (3)	C8—C13	1.408 (6)
Er2—O7^{iii}	2.256 (3)	C8—C20	1.505 (6)
Er2—O7^{i}	2.256 (3)	C9—C10	1.393 (7)
Er2—O3	2.353 (3)	C9—H9A	0.9300
Er2—O3^{ii}	2.353 (3)	C10—C11	1.376 (8)
Er2—O4^{ii}	2.563 (3)	C10—H10A	0.9300
Er2—O4	2.563 (3)	C11—C12	1.384 (7)
Er2—C20	2.817 (5)	C11—H11A	0.9300
Er2—C20^{ii}	2.817 (5)	C12—C13	1.399 (6)
O1—C7	1.248 (5)	C12—H12A	0.9300
O2—C7	1.253 (5)	C13—C14	1.485 (6)
O3—C20	1.244 (5)	C14—C15	1.396 (6)
O4—C20	1.275 (5)	C14—C19	1.410 (6)
O6—C21	1.255 (5)	C15—C16	1.374 (7)
O7—C21	1.263 (5)	C15—H15A	0.9300
O7—Er2^{iv}	2.256 (3)	C16—C17	1.378 (7)
O5—H5A	0.8501	C16—H16A	0.9300

O5—H5C	0.8499	C17—C18	1.376 (6)
C1—C6	1.391 (6)	C17—H17A	0.9300
C1—C2	1.403 (6)	C18—C19	1.387 (6)
C1—C7	1.516 (6)	C18—H18A	0.9300
C2—C3	1.406 (6)	C19—C21	1.500 (5)
O6—Er1—O6^{i}	87.60 (15)	C20—O3—Er2	98.4 (3)
O6—Er1—O4^{i}	77.96 (10)	C20—O4—Er1	135.9 (3)
O6^{i}—Er1—O4^{i}	72.81 (10)	C20—O4—Er2	87.7 (3)
O6—Er1—O4	72.81 (10)	Er1—O4—Er2	124.72 (12)
O6^{i}—Er1—O4	77.96 (10)	C21—O6—Er1	142.2 (3)
O4^{i}—Er1—O4	139.12 (14)	C21—O7—Er2^{iv}	137.0 (3)
O6—Er1—O1	146.49 (10)	Er1—O5—H5A	120.0
O6^{i}—Er1—O1	90.54 (11)	Er1—O5—H5C	120.0
O4^{i}—Er1—O1	133.02 (10)	H5A—O5—H5C	120.0
O4—Er1—O1	74.08 (10)	C6—C1—C2	119.4 (4)
O6—Er1—O1^{i}	90.54 (11)	C6—C1—C7	116.8 (4)
O6^{i}—Er1—O1^{i}	146.49 (10)	C2—C1—C7	123.8 (4)
O4^{i}—Er1—O1^{i}	74.08 (10)	C1—C2—C3	118.5 (4)
O4—Er1—O1^{i}	133.02 (10)	C1—C2—C2^{ii}	122.5 (3)
O1—Er1—O1^{i}	108.51 (14)	C3—C2—C2^{ii}	119.0 (3)
O6—Er1—O5	147.08 (11)	C4—C3—C2	120.9 (4)
O6^{i}—Er1—O5	93.51 (12)	C4—C3—H3A	119.5
O4^{i}—Er1—O5	71.04 (10)	C2—C3—H3A	119.5
O4—Er1—O5	139.53 (10)	C5—C4—C3	120.5 (5)
O1—Er1—O5	66.43 (10)	C5—C4—H4A	119.8
O1^{i}—Er1—O5	70.78 (11)	C3—C4—H4A	119.8
O6—Er1—O5^{i}	93.51 (12)	C4—C5—C6	119.3 (5)
O6^{i}—Er1—O5^{i}	147.08 (11)	C4—C5—H5B	120.3
O4^{i}—Er1—O5^{i}	139.53 (10)	C6—C5—H5B	120.3
O4—Er1—O5^{i}	71.04 (10)	C5—C6—C1	121.4 (4)
O1—Er1—O5^{i}	70.78 (11)	C5—C6—H6A	119.3
O1^{i}—Er1—O5^{i}	66.43 (10)	C1—C6—H6A	119.3
O5—Er1—O5^{i}	102.79 (17)	O1—C7—O2	125.2 (4)
O2—Er2—O2^{ii}	81.52 (14)	O1—C7—C1	119.0 (4)
O2—Er2—O7^{iii}	149.88 (11)	O2—C7—C1	115.7 (4)
O2^{ii}—Er2—O7^{iii}	88.36 (11)	C9—C8—C13	120.3 (5)
O2—Er2—O7^{i}	88.36 (11)	C9—C8—C20	117.0 (4)
O2^{ii}—Er2—O7^{i}	149.88 (11)	C13—C8—C20	122.4 (4)
O7^{iii}—Er2—O7^{i}	112.99 (15)	C8—C9—C10	121.3 (5)
O2—Er2—O3	130.55 (11)	C8—C9—H9A	119.3
O2^{ii}—Er2—O3	85.16 (11)	C10—C9—H9A	119.3
O7^{iii}—Er2—O3	76.13 (11)	C11—C10—C9	118.5 (5)

O7^{i}—Er2—O3	80.06 (11)	C11—C10—H10A	120.8
O2—Er2—O3^{ii}	85.16 (11)	C9—C10—H10A	120.8
O2^{ii}—Er2—O3^{ii}	130.55 (11)	C10—C11—C12	121.0 (5)
O7^{iii}—Er2—O3^{ii}	80.06 (11)	C10—C11—H11A	119.5
O7^{i}—Er2—O3^{ii}	76.13 (11)	C12—C11—H11A	119.5
O3—Er2—O3^{ii}	136.14 (15)	C11—C12—C13	121.2 (5)
O2—Er2—O4^{ii}	73.76 (10)	C11—C12—H12A	119.4
O2^{ii}—Er2—O4^{ii}	77.94 (10)	C13—C12—H12A	119.4
O7^{iii}—Er2—O4^{ii}	76.40 (10)	C12—C13—C8	117.6 (4)
O7^{i}—Er2—O4^{ii}	126.24 (10)	C12—C13—C14	118.0 (4)
O3—Er2—O4^{ii}	148.00 (10)	C8—C13—C14	124.2 (4)
O3^{ii}—Er2—O4^{ii}	52.62 (9)	C15—C14—C19	117.3 (4)
O2—Er2—O4	77.94 (10)	C15—C14—C13	117.4 (4)
O2^{ii}—Er2—O4	73.76 (10)	C19—C14—C13	125.1 (4)
O7^{iii}—Er2—O4	126.24 (10)	C16—C15—C14	122.5 (5)
O7^{i}—Er2—O4	76.40 (10)	C16—C15—H15A	118.8
O3—Er2—O4	52.62 (9)	C14—C15—H15A	118.8
O3^{ii}—Er2—O4	148.00 (10)	C15—C16—C17	119.8 (5)
O4^{ii}—Er2—O4	142.37 (13)	C15—C16—H16A	120.1
O2—Er2—C20	104.77 (12)	C17—C16—H16A	120.1
O2^{ii}—Er2—C20	76.29 (11)	C16—C17—C18	119.0 (5)
O7^{iii}—Er2—C20	100.19 (12)	C16—C17—H17A	120.5
O7^{i}—Er2—C20	79.05 (12)	C18—C17—H17A	120.5
O3—Er2—C20	25.90 (10)	C17—C18—C19	122.2 (5)
O3^{ii}—Er2—C20	152.97 (11)	C17—C18—H18A	118.9
O4^{ii}—Er2—C20	154.10 (10)	C19—C18—H18A	118.9
O4—Er2—C20	26.89 (10)	C18—C19—C14	119.2 (4)
O2—Er2—C20^{ii}	76.29 (11)	C18—C19—C21	117.0 (4)
O2^{ii}—Er2—C20^{ii}	104.77 (12)	C14—C19—C21	123.6 (4)
O7^{iii}—Er2—C20^{ii}	79.05 (12)	O3—C20—O4	120.5 (4)
O7^{i}—Er2—C20^{ii}	100.19 (12)	O3—C20—C8	118.1 (4)
O3—Er2—C20^{ii}	152.97 (11)	O4—C20—C8	121.0 (4)
O3^{ii}—Er2—C20^{ii}	25.90 (10)	O3—C20—Er2	55.7 (2)
O4^{ii}—Er2—C20^{ii}	26.89 (10)	O4—C20—Er2	65.4 (2)
O4—Er2—C20^{ii}	154.10 (10)	C8—C20—Er2	164.9 (3)
C20—Er2—C20^{ii}	178.64 (17)	O6—C21—O7	124.1 (4)
C7—O1—Er1	133.4 (3)	O6—C21—C19	119.7 (4)
C7—O2—Er2	135.3 (3)	O7—C21—C19	116.2 (4)

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

Fig. 1

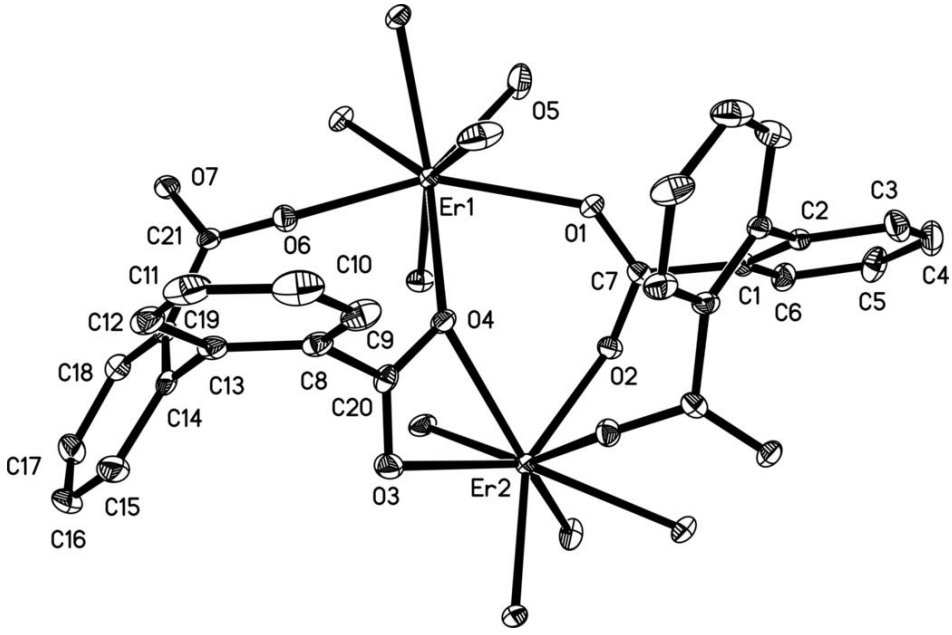
O5
O7
Er1
C21
O6
O1
C3
C2
C11
C10
C7
C4
C1
C6
C5
C12
C19
O4
C9
C18
C13
C8
O2
C20
C14
C17
O3
Er2
C15
C16

Fig. 2