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1,3-Diisopropylimidazolium bis(cyclooctatetraenyl)erbate(III)

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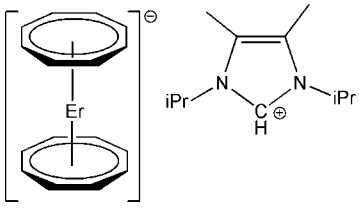
Key indicators: single-crystal X-ray study; T = 133 K; mean σ(C–C) = 0.003 Å; R factor = 0.020; wR factor = 0.042; data-to-parameter ratio = 26.1.

In the title compound, $(C_{11}H_{21}N_2)[Er(C_8H_8)_2]$, the anion displays the sandwich form with planar and parallel cyclooctatetraenyl ligands. The perpendicular distances of the Er atom from the C_8 planes are 1.8809 (7) and 1.8476 (8) Å, with individual Er—C bond lengths in the range 2.596 (2)–2.651 (2) Å. The extended structure consists of chains of alternating anions and cations parallel to (101); residues are connected by C—H$\cdots\pi$ interactions and neighbouring formula units are related by an n glide plane.

Related literature

For related literature, see: Arduengo *et al.* (1991); Boussie *et al.* (1991); Hayes & Thomas (1969); Hodgson *et al.* (1973); Mares *et al.*, (1970); Schumann *et al.* (1985, 1993); Streitwieser & Müller-Westerhoff (1968); Xia *et al.* (1991).



Experimental

Crystal data

$(C_{11}H_{21}N_2)[Er(C_8H_8)_2]$
M_r = 556.85
Monoclinic, $P2_1/n$
a = 12.7879 (12) Å
b = 8.7333 (8) Å
c = 21.531 (2) Å
β = 94.100 (3)°
V = 2398.5 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.51 mm^{-1}
T = 133 (2) K
0.33 × 0.25 × 0.14 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.390, T_{max} = 0.639
46432 measured reflections
7325 independent reflections
6213 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.020
$wR(F^2)$ = 0.042
S = 1.11
7325 reflections
281 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.88 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Er—C11	2.596 (2)	Er—C8	2.627 (2)
Er—C13	2.599 (2)	Er—C6	2.627 (2)
Er—C10	2.600 (2)	Er—C1	2.633 (2)
Er—C15	2.600 (2)	Er—C4	2.634 (2)
Er—C14	2.602 (2)	Er—C2	2.636 (2)
Er—C12	2.602 (2)	Er—C7	2.636 (2)
Er—C5	2.6080 (19)	Er—C3	2.651 (2)
Er—C16	2.611 (2)	N1—C17	1.330 (3)
Er—C9	2.615 (2)	N2—C17	1.335 (2)
N1—C17—N2	109.26 (17)		

Table 2
C—H$\cdots\pi$ interactions (Å, °).

D—H$\cdots A$	Distance H$\cdots A$	Angle D—H$\cdots A$	Symmetry code
C25—H25$\cdots Cg$(C1–C8)	2.27	178	
C17—H17$\cdots$Cent(C4—C5)	2.33	169	
C20—H20$\cdots$Cent(C10—C11)	2.58	140	$(\frac{1}{2}+x, \frac{1}{2}-y, \frac{1}{2}+z)$
C22—H22$C\cdots$Cent(C12—C13)	2.67	151	$(\frac{1}{2}+x, \frac{1}{2}-y, \frac{1}{2}+z)$

Notes: C—H distances are normalized to 1.08Å, Cg is the centre of gravity of a ring and Cent is the mid-point of a bond.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* (Siemens, 1994); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2409).

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supplementary materials

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1,3-Diisopropylimidazolium bis(cyclooctatetraenyl)erbate(III)

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Comment

After the synthesis of uranocene [$(COT)_2U$] (COT = cyclooctatetraenyl, $(C_8H_8)^{2-}$) by Streitwieser & Müller-Westerhoff (1968), bis-cyclooctatetraene complexes of divalent lanthanides were reported by Hayes & Thomas (1969). Streitwieser isolated trivalent lanthanide complexes of the type [$K(COT)_2Ln$] (Ln = Y, La, Ce, Pr, Nd, Sm, Gd, Tb) (Mares *et al.*, 1970; Streitwieser *et al.*, 1973; Hodgson *et al.*, 1973) using the same methodology as for the preparation of uranocene. Later, [$K(COT)_2Ln$] complexes of ytterbium (Boussie *et al.*, 1991) and lutetium (Schumann *et al.*, 1993) were reported. In 1991 Chen synthesized an erbium complex with a tetralayer sandwich structure in which the adjacent Er^{3+} and K^+ ions are bridged by η^8-cyclooctatetraenyl groups (Xia *et al.*, 1991). Here we report the anionic mononuclear sandwich complex of bis(cyclooctatetraenyl)erbium(III) with the carbenium cation 1,3- diisopropylimidazolium (Fig. 1).

The compound crystallizes without imposed symmetry. The coordination polyhedron is formed by two planar eight-membered rings (r.m.s. deviation 0.016, 0.006 Å) in an almost parallel arrangement with an interplanar angle of 2.21 (9)°. The perpendicular distances of the Er atom from the C_8 planes are 1.8809 (7) and 1.8476 (8) Å. The angle cent1—Er—cent2 (cent = centroid) is 178°. The rings are eclipsed, as shown by torsion angles, *e.g.* C1—*Cg*1—*Cg*2—C12 = −3°, where *Cg* are ring centres of gravity. The individual Er—C bond lengths range from 2.596 (2)–2.651 (2) Å, which is comparable with Er—C(η^8) [2.569 (14)–2.660 (19) Å], Er—C(η^5) [2.629 (15)–2.654 (13) Å] reported for (COT)Er(μ-COT)K(μ-COT)Er(μ-COT)K$(THF)_4$ (Xia *et al.* 1991), and (μ^5-$C_5H_5)_2$Er(μ-$CH_3)_2$Li(tmeda) (tmeda = tetramethylethylenediamine) (Schumann *et al.* 1985) respectively. In the imidazolium ion, the N—C distances [1.330 (3) and 1.335 (2) Å] are slightly shorter than those of 1,3-di(1-adamantyl)imidazol-2-ylidene reported by Arduengo *et al.* (1991) [1.367 (2) and 1.373 (2) Å], indicating delocalization of the positive charge over the N1—C17—N2 unit.

The packing involves several short interionic ("charge-assisted") contacts, principally from the more acidic H atoms H17, H20 and H25 (but also from H22C). The C—H bond distances were normalized to 1.08Å to calculate the contact distances. The shortest is from H25 to the centroid of C1–8, with H···cent 2.27 Å, C—H···cent 178°. The other contacts are best described as involving individual bonds as acceptors: C17—H17···C4,C5 [H···C 2.55, 2.31 Å, angles 156, 165°]; C20—H20···C10,C11 [2.73, 2.62 Å, 143, 133°, operator 1/2 + *x*, 1/2 − *y*, 1/2 + *z*]; C22—H22C—C12,C13 [2.80, 2.73 Å, 138, 163°, same operator]. The net effect is to connect the residues to form a chain parallel to (101) (Fig. 2). Between chains, a short C22···C22 contact is observed [3.168 (4) Å, operator 1 − *x*,1 − *y*,1 − *z*].

Experimental

The title compound was crystallized from THF/pentane by the reaction of $ErCl_3$, 1,3 diisopropylimidazolin-2-ylidene and freshly prepared K_2COT and by subsequent extraction and filtration from toluene. Elemental analysis: $C_{27}H_{37}ErN_2$ (556.85 g/mol), Calculated: C 58.23, H 6.69, N 5.03; Found C 58.01, H 6.10, N 5.45%.

Refinement

Methyl hydrogen atoms were located in a difference synthesis; the methyl groups were idealized and refined as rigid groups allowed to rotate but not tip, with C—H 0.98 Å, H—C—H 109.5°. Atom H17 was freely refined [C17—H17 refined to 0.91 (2) Å]. Other hydrogen atoms were included using a riding model with C—H 0.95 (aromatic), 1.00 (methylidyne) Å; U(H) values were fixed at 1.2U(C) of the parent C atom.

The two difference peaks larger than 1 e $Å^{-3}$ are not located near the Er atom, but instead lie 1.12 Å from H1 and 1.89 Å from H27A, respectively. Since the largest peak has *x* and *z* coordinates equal to those of Er, we tentatively ascribe these peaks to the effect of a small unidentified twinning component.

In the supplementary material, the extremely long list of torsion angles involving the Er atom has been omitted.

Figures

Fig. 1. The formula unit of the title compound in the crystal. Ellipsoids represent 30% probability levels.

Fig. 2. Chain formation *via* short C—H···π contacts (thin dashed bonds) - see text. H atoms not involved in short contacts are omitted for clarity.

1,3-Diisopropylimidazolium bis(cyclooctatetraenyl)erbate(III)

Crystal data

$(C_{11}H_{21}N_2)[Er(C_8H_8)_2]$	F_{000} = 1124
M_r = 556.85	D_x = 1.542 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 12.7879 (12) Å	Cell parameters from 7131 reflections
b = 8.7333 (8) Å	θ = 2–30º
c = 21.531 (2) Å	μ = 3.51 mm^{-1}
β = 94.100 (3)º	*T* = 133 (2) K
V = 2398.5 (4) $Å^3$	Tablet, yellow
Z = 4	0.33 × 0.25 × 0.14 mm

Data collection

Bruker SMART 1000 CCD	7325 independent reflections

diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

Detector resolution: 8.192 pixels mm^{-1}

T = 133(2) K

ω and φ scans

Absorption correction: multi-scan (SADABS; Bruker, 1998)

T_{min} = 0.390, T_{max} = 0.639

46432 measured reflections

6213 reflections with $I > 2\sigma(I)$

R_{int} = 0.031

θ_{max} = 30.5º

θ_{min} = 1.8º

$h = -18 \rightarrow 18$

$k = -12 \rightarrow 12$

$l = -30 \rightarrow 30$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.020

$wR(F^2)$ = 0.042

S = 1.11

7325 reflections

281 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0093P)^2 + 2.7708P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max}$ = 0.002

$\Delta\rho_{max}$ = 1.24 e $Å^{-3}$

$\Delta\rho_{min}$ = −0.88 e $Å^{-3}$

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 $F^2 > 2$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}
Er	0.294863 (6)	0.393357 (10)	0.098885 (4)	0.01441 (3)
N1	0.59507 (12)	0.71121 (19)	0.27630 (7)	0.0149 (3)
N2	0.62422 (13)	0.5389 (2)	0.34830 (7)	0.0163 (3)
C1	0.36080 (18)	0.6787 (3)	0.09668 (10)	0.0250 (4)
H1	0.3470	0.7621	0.0690	0.030*
C2	0.29094 (17)	0.6728 (3)	0.14489 (10)	0.0244 (4)
H2	0.2409	0.7533	0.1420	0.029*

C3	0.27823 (17)	0.5760 (3)	0.19602 (10)	0.0237 (4)
H3	0.2237	0.6094	0.2205	0.028*
C4	0.32684 (17)	0.4418 (3)	0.21950 (9)	0.0228 (4)
H4	0.2963	0.4046	0.2555	0.027*
C5	0.41019 (17)	0.3494 (3)	0.20220 (9)	0.0223 (4)
H5	0.4204	0.2616	0.2279	0.027*
C6	0.48199 (16)	0.3570 (3)	0.15561 (10)	0.0237 (4)
H6	0.5318	0.2761	0.1586	0.028*
C7	0.49692 (16)	0.4567 (3)	0.10561 (10)	0.0244 (4)
H7	0.5553	0.4284	0.0832	0.029*
C8	0.44589 (17)	0.5887 (3)	0.08083 (9)	0.0249 (5)
H8	0.4764	0.6256	0.0448	0.030*
C9	0.30900 (18)	0.1185 (3)	0.05205 (12)	0.0314 (5)
H9	0.3603	0.0396	0.0535	0.038*
C10	0.31984 (18)	0.2205 (3)	0.00278 (11)	0.0318 (6)
H10	0.3780	0.1962	−0.0205	0.038*
C11	0.2650 (2)	0.3504 (3)	−0.02038 (10)	0.0315 (6)
H11	0.2944	0.3931	−0.0558	0.038*
C12	0.1758 (2)	0.4324 (3)	−0.00302 (11)	0.0329 (6)
H12	0.1585	0.5166	−0.0297	0.040*
C13	0.10714 (18)	0.4170 (3)	0.04490 (12)	0.0330 (6)
H13	0.0544	0.4938	0.0431	0.040*
C14	0.09810 (17)	0.3154 (3)	0.09458 (11)	0.0326 (6)
H14	0.0405	0.3393	0.1184	0.039*
C15	0.15398 (19)	0.1868 (3)	0.11750 (10)	0.0314 (5)
H15	0.1263	0.1457	0.1537	0.038*
C16	0.2406 (2)	0.1052 (3)	0.09965 (11)	0.0321 (5)
H16	0.2571	0.0202	0.1261	0.038*
C17	0.56693 (15)	0.5738 (2)	0.29595 (9)	0.0163 (4)
H17	0.5164 (17)	0.515 (3)	0.2758 (10)	0.015 (6)*
C18	0.69194 (15)	0.6603 (2)	0.36310 (9)	0.0184 (4)
C19	0.67409 (15)	0.7684 (2)	0.31794 (9)	0.0183 (4)
C20	0.61502 (16)	0.3970 (2)	0.38588 (9)	0.0193 (4)
H20	0.6873	0.3609	0.3994	0.023*
C21	0.5605 (2)	0.2722 (3)	0.34720 (11)	0.0332 (6)
H21A	0.5639	0.1759	0.3706	0.040*
H21B	0.5951	0.2593	0.3084	0.040*
H21C	0.4869	0.3005	0.3375	0.040*
C22	0.55787 (19)	0.4316 (3)	0.44359 (10)	0.0284 (5)
H22A	0.4867	0.4670	0.4312	0.034*
H22B	0.5956	0.5116	0.4680	0.034*
H22C	0.5544	0.3386	0.4688	0.034*
C23	0.76721 (18)	0.6623 (3)	0.41938 (10)	0.0271 (5)
H23A	0.8244	0.7338	0.4127	0.033*
H23B	0.7959	0.5594	0.4268	0.033*
H23C	0.7307	0.6952	0.4556	0.033*
C24	0.72744 (18)	0.9190 (3)	0.31202 (11)	0.0277 (5)
H24A	0.7691	0.9422	0.3509	0.033*
H24B	0.6747	0.9992	0.3037	0.033*

H24C	0.7736	0.9145	0.2776	0.033*
C25	0.54317 (15)	0.7822 (2)	0.21896 (8)	0.0172 (4)
H25	0.4951	0.7030	0.1992	0.021*
C26	0.47505 (18)	0.9167 (3)	0.23510 (10)	0.0266 (5)
H26A	0.4251	0.8836	0.2649	0.032*
H26B	0.4366	0.9547	0.1972	0.032*
H26C	0.5194	0.9986	0.2537	0.032*
C27	0.62160 (18)	0.8210 (3)	0.17196 (10)	0.0269 (5)
H27A	0.6652	0.9072	0.1874	0.032*
H27B	0.5842	0.8491	0.1323	0.032*
H27C	0.6663	0.7319	0.1658	0.032*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Er	0.01515 (4)	0.01363 (4)	0.01403 (4)	−0.00244 (3)	−0.00180 (3)	−0.00117 (3)
N1	0.0138 (7)	0.0175 (9)	0.0131 (7)	0.0002 (6)	−0.0003 (6)	−0.0001 (6)
N2	0.0180 (8)	0.0165 (9)	0.0144 (7)	0.0017 (6)	0.0010 (6)	0.0011 (6)
C1	0.0349 (12)	0.0153 (11)	0.0233 (10)	−0.0087 (9)	−0.0080 (8)	0.0038 (8)
C2	0.0253 (10)	0.0131 (10)	0.0338 (11)	0.0011 (8)	−0.0051 (8)	−0.0051 (9)
C3	0.0225 (10)	0.0231 (12)	0.0261 (10)	−0.0023 (8)	0.0050 (8)	−0.0114 (8)
C4	0.0283 (11)	0.0260 (11)	0.0140 (9)	−0.0095 (8)	0.0015 (8)	−0.0027 (8)
C5	0.0267 (10)	0.0204 (11)	0.0185 (9)	−0.0046 (8)	−0.0074 (8)	0.0030 (7)
C6	0.0178 (9)	0.0241 (12)	0.0281 (11)	0.0021 (7)	−0.0065 (8)	−0.0041 (8)
C7	0.0169 (9)	0.0325 (13)	0.0241 (10)	−0.0056 (8)	0.0029 (8)	−0.0085 (9)
C8	0.0270 (10)	0.0315 (13)	0.0161 (9)	−0.0143 (9)	0.0019 (8)	−0.0009 (8)
C9	0.0290 (11)	0.0196 (12)	0.0436 (13)	0.0023 (9)	−0.0105 (10)	−0.0143 (10)
C10	0.0243 (11)	0.0421 (15)	0.0294 (12)	−0.0097 (10)	0.0048 (9)	−0.0209 (10)
C11	0.0416 (13)	0.0385 (15)	0.0141 (9)	−0.0209 (11)	0.0003 (9)	−0.0033 (9)
C12	0.0449 (14)	0.0247 (13)	0.0259 (11)	−0.0077 (10)	−0.0206 (10)	0.0057 (9)
C13	0.0233 (11)	0.0341 (15)	0.0390 (13)	0.0075 (9)	−0.0171 (9)	−0.0121 (10)
C14	0.0173 (10)	0.0508 (16)	0.0299 (12)	−0.0090 (10)	0.0026 (8)	−0.0164 (11)
C15	0.0319 (12)	0.0390 (15)	0.0230 (10)	−0.0221 (11)	−0.0002 (9)	0.0021 (10)
C16	0.0418 (13)	0.0190 (11)	0.0328 (12)	−0.0137 (10)	−0.0150 (10)	0.0057 (10)
C17	0.0163 (9)	0.0172 (10)	0.0153 (8)	0.0006 (7)	0.0011 (7)	−0.0003 (7)
C18	0.0178 (9)	0.0189 (10)	0.0179 (9)	0.0021 (7)	−0.0019 (7)	−0.0016 (7)
C19	0.0161 (9)	0.0192 (10)	0.0192 (9)	−0.0006 (7)	−0.0024 (7)	−0.0025 (7)
C20	0.0225 (9)	0.0177 (10)	0.0175 (8)	0.0032 (8)	−0.0002 (7)	0.0056 (8)
C21	0.0511 (15)	0.0224 (13)	0.0252 (11)	−0.0061 (10)	−0.0046 (10)	0.0058 (9)
C22	0.0321 (12)	0.0323 (14)	0.0217 (10)	0.0089 (9)	0.0088 (9)	0.0071 (9)
C23	0.0295 (11)	0.0265 (12)	0.0234 (10)	−0.0016 (9)	−0.0114 (8)	−0.0001 (9)
C24	0.0272 (11)	0.0239 (13)	0.0303 (11)	−0.0079 (9)	−0.0092 (9)	0.0027 (9)
C25	0.0189 (9)	0.0192 (10)	0.0129 (8)	−0.0014 (7)	−0.0029 (7)	0.0010 (7)
C26	0.0272 (11)	0.0268 (13)	0.0250 (10)	0.0090 (9)	−0.0041 (8)	0.0005 (9)
C27	0.0308 (11)	0.0316 (13)	0.0186 (10)	−0.0040 (10)	0.0043 (8)	0.0035 (9)

Geometric parameters (Å, °)

Er—C11	2.596 (2)	C10—C11	1.407 (4)

Er—C13	2.599 (2)	C10—H10	0.9500
Er—C10	2.600 (2)	C11—C12	1.419 (4)
Er—C15	2.600 (2)	C11—H11	0.9500
Er—C14	2.602 (2)	C12—C13	1.408 (4)
Er—C12	2.602 (2)	C12—H12	0.9500
Er—C5	2.6080 (19)	C13—C14	1.401 (4)
Er—C16	2.611 (2)	C13—H13	0.9500
Er—C9	2.615 (2)	C14—C15	1.402 (4)
Er—C8	2.627 (2)	C14—H14	0.9500
Er—C6	2.627 (2)	C15—C16	1.395 (4)
Er—C1	2.633 (2)	C15—H15	0.9500
Er—C4	2.634 (2)	C16—H16	0.9500
Er—C2	2.636 (2)	C17—H17	0.91 (2)
Er—C7	2.636 (2)	C18—C19	1.363 (3)
Er—C3	2.651 (2)	C18—C23	1.493 (3)
N1—C17	1.330 (3)	C19—C24	1.491 (3)
N1—C19	1.395 (2)	C20—C21	1.512 (3)
N1—C25	1.494 (2)	C20—C22	1.516 (3)
N2—C17	1.335 (2)	C20—H20	1.0000
N2—C18	1.391 (3)	C21—H21A	0.9800
N2—C20	1.489 (3)	C21—H21B	0.9800
C1—C8	1.404 (3)	C21—H21C	0.9800
C1—C2	1.418 (3)	C22—H22A	0.9800
C1—H1	0.9500	C22—H22B	0.9800
C2—C3	1.407 (3)	C22—H22C	0.9800
C2—H2	0.9500	C23—H23A	0.9800
C3—C4	1.404 (3)	C23—H23B	0.9800
C3—H3	0.9500	C23—H23C	0.9800
C4—C5	1.408 (3)	C24—H24A	0.9800
C4—H4	0.9500	C24—H24B	0.9800
C5—C6	1.409 (3)	C24—H24C	0.9800
C5—H5	0.9500	C25—C27	1.513 (3)
C6—C7	1.409 (3)	C25—C26	1.517 (3)
C6—H6	0.9500	C25—H25	1.0000
C7—C8	1.411 (3)	C26—H26A	0.9800
C7—H7	0.9500	C26—H26B	0.9800
C8—H8	0.9500	C26—H26C	0.9800
C9—C16	1.399 (4)	C27—H27A	0.9800
C9—C10	1.399 (4)	C27—H27B	0.9800
C9—H9	0.9500	C27—H27C	0.9800
C11—Er—C13	60.21 (8)	C2—C3—Er	73.97 (12)
C11—Er—C10	31.42 (8)	C4—C3—H3	112.4
C13—Er—C10	81.51 (8)	C2—C3—H3	112.4
C11—Er—C15	89.87 (7)	Er—C3—H3	136.6
C13—Er—C15	59.75 (8)	C3—C4—C5	135.0 (2)
C10—Er—C15	81.13 (8)	C3—C4—Er	75.25 (12)
C11—Er—C14	81.57 (7)	C5—C4—Er	73.40 (11)
C13—Er—C14	31.25 (8)	C3—C4—H4	112.5
C10—Er—C14	89.61 (7)	C5—C4—H4	112.5

C15—Er—C14	31.26 (9)	Er—C4—H4	134.9
C11—Er—C12	31.69 (9)	C4—C5—C6	134.9 (2)
C13—Er—C12	31.40 (8)	C4—C5—Er	75.45 (11)
C10—Er—C12	60.18 (8)	C6—C5—Er	75.13 (11)
C15—Er—C12	81.41 (8)	C4—C5—H5	112.6
C14—Er—C12	59.87 (8)	C6—C5—H5	112.6
C11—Er—C5	148.95 (8)	Er—C5—H5	131.5
C13—Er—C5	147.24 (8)	C7—C6—C5	134.7 (2)
C10—Er—C5	119.96 (8)	C7—C6—Er	74.84 (12)
C15—Er—C5	97.02 (7)	C5—C6—Er	73.64 (11)
C14—Er—C5	118.58 (7)	C7—C6—H6	112.6
C12—Er—C5	178.40 (7)	C5—C6—H6	112.6
C11—Er—C16	81.18 (8)	Er—C6—H6	134.9
C13—Er—C16	80.92 (8)	C6—C7—C8	135.3 (2)
C10—Er—C16	59.54 (8)	C6—C7—Er	74.11 (12)
C15—Er—C16	31.04 (8)	C8—C7—Er	74.08 (12)
C14—Er—C16	59.42 (9)	C6—C7—H7	112.4
C12—Er—C16	89.53 (7)	C8—C7—H7	112.4
C5—Er—C16	89.27 (7)	Er—C7—H7	136.1
C11—Er—C9	59.69 (8)	C1—C8—C7	135.3 (2)
C13—Er—C9	89.29 (7)	C1—C8—Er	74.75 (12)
C10—Er—C9	31.13 (8)	C7—C8—Er	74.83 (12)
C15—Er—C9	59.37 (8)	C1—C8—H8	112.3
C14—Er—C9	80.76 (8)	C7—C8—H8	112.3
C12—Er—C9	81.23 (8)	Er—C8—H8	133.7
C5—Er—C9	98.25 (7)	C16—C9—C10	135.2 (2)
C16—Er—C9	31.06 (8)	C16—C9—Er	74.33 (14)
C11—Er—C8	90.30 (7)	C10—C9—Er	73.84 (14)
C13—Er—C8	123.19 (8)	C16—C9—H9	112.4
C10—Er—C8	97.24 (7)	C10—C9—H9	112.4
C15—Er—C8	176.50 (8)	Er—C9—H9	136.0
C14—Er—C8	152.13 (8)	C9—C10—C11	135.1 (2)
C12—Er—C8	100.51 (7)	C9—C10—Er	75.03 (13)
C5—Er—C8	81.08 (7)	C11—C10—Er	74.16 (13)
C16—Er—C8	145.65 (8)	C9—C10—H10	112.5
C9—Er—C8	117.87 (8)	C11—C10—H10	112.5
C11—Er—C6	120.48 (8)	Er—C10—H10	134.1
C13—Er—C6	177.29 (8)	C10—C11—C12	134.7 (2)
C10—Er—C6	98.05 (7)	C10—C11—Er	74.43 (12)
C15—Er—C6	117.55 (8)	C12—C11—Er	74.38 (12)
C14—Er—C6	146.24 (8)	C10—C11—H11	112.6
C12—Er—C6	150.07 (8)	C12—C11—H11	112.6
C5—Er—C6	31.23 (7)	Er—C11—H11	134.3
C16—Er—C6	96.55 (7)	C13—C12—C11	134.4 (2)
C9—Er—C6	88.99 (7)	C13—C12—Er	74.19 (12)
C8—Er—C6	59.50 (7)	C11—C12—Er	73.93 (12)
C11—Er—C1	98.26 (7)	C13—C12—H12	112.8
C13—Er—C1	101.73 (8)	C11—C12—H12	112.8
C10—Er—C1	118.54 (8)	Er—C12—H12	135.2

C15—Er—C1	152.33 (8)	C14—C13—C12	135.2 (2)
C14—Er—C1	123.86 (8)	C14—C13—Er	74.47 (12)
C12—Er—C1	91.70 (7)	C12—C13—Er	74.40 (13)
C5—Er—C1	89.56 (6)	C14—C13—H13	112.4
C16—Er—C1	176.61 (8)	C12—C13—H13	112.4
C9—Er—C1	146.21 (8)	Er—C13—H13	134.8
C8—Er—C1	30.97 (7)	C13—C14—C15	135.1 (2)
C6—Er—C1	80.83 (7)	C13—C14—Er	74.28 (13)
C11—Er—C4	178.95 (7)	C15—C14—Er	74.31 (12)
C13—Er—C4	120.09 (8)	C13—C14—H14	112.4
C10—Er—C4	149.18 (8)	C15—C14—H14	112.4
C15—Er—C4	91.13 (7)	Er—C14—H14	135.1
C14—Er—C4	99.13 (7)	C16—C15—C14	135.1 (2)
C12—Er—C4	148.26 (8)	C16—C15—Er	74.91 (13)
C5—Er—C4	31.15 (7)	C14—C15—Er	74.43 (13)
C16—Er—C4	99.85 (7)	C16—C15—H15	112.5
C9—Er—C4	121.16 (8)	C14—C15—H15	112.5
C8—Er—C4	88.72 (6)	Er—C15—H15	133.8
C6—Er—C4	59.27 (7)	C15—C16—C9	135.2 (2)
C1—Er—C4	80.70 (7)	C15—C16—Er	74.05 (14)
C11—Er—C2	120.00 (8)	C9—C16—Er	74.61 (14)
C13—Er—C2	93.02 (7)	C15—C16—H16	112.4
C10—Er—C2	147.53 (8)	C9—C16—H16	112.4
C15—Er—C2	123.52 (8)	Er—C16—H16	135.1
C14—Er—C2	102.20 (8)	N1—C17—N2	109.26 (17)
C12—Er—C2	99.78 (7)	N1—C17—H17	124.0 (14)
C5—Er—C2	80.82 (7)	N2—C17—H17	126.8 (14)
C16—Er—C2	151.40 (8)	C19—C18—N2	107.14 (16)
C9—Er—C2	177.00 (7)	C19—C18—C23	129.5 (2)
C8—Er—C2	59.21 (7)	N2—C18—C23	123.35 (18)
C6—Er—C2	88.77 (7)	C18—C19—N1	106.68 (18)
C1—Er—C2	31.23 (7)	C18—C19—C24	128.14 (18)
C4—Er—C2	59.11 (7)	N1—C19—C24	125.18 (18)
C11—Er—C7	99.16 (7)	N2—C20—C21	110.60 (16)
C13—Er—C7	151.40 (8)	N2—C20—C22	109.92 (17)
C10—Er—C7	89.42 (7)	C21—C20—C22	111.38 (19)
C15—Er—C7	145.51 (8)	N2—C20—H20	108.3
C14—Er—C7	176.77 (8)	C21—C20—H20	108.3
C12—Er—C7	122.08 (8)	C22—C20—H20	108.3
C5—Er—C7	59.45 (7)	C20—C21—H21A	109.5
C16—Er—C7	117.51 (8)	C20—C21—H21B	109.5
C9—Er—C7	96.86 (7)	H21A—C21—H21B	109.5
C8—Er—C7	31.09 (7)	C20—C21—H21C	109.5
C6—Er—C7	31.04 (7)	H21A—C21—H21C	109.5
C1—Er—C7	59.23 (7)	H21B—C21—H21C	109.5
C4—Er—C7	80.19 (7)	C20—C22—H22A	109.5
C2—Er—C7	80.20 (7)	C20—C22—H22B	109.5
C11—Er—C3	148.53 (8)	H22A—C22—H22B	109.5
C13—Er—C3	100.45 (7)	C20—C22—H22C	109.5

C10—Er—C3	177.23 (7)	H22A—C22—H22C	109.5
C15—Er—C3	101.54 (7)	H22B—C22—H22C	109.5
C14—Er—C3	93.07 (7)	C18—C23—H23A	109.5
C12—Er—C3	120.75 (8)	C18—C23—H23B	109.5
C5—Er—C3	59.19 (7)	H23A—C23—H23B	109.5
C16—Er—C3	122.59 (8)	C18—C23—H23C	109.5
C9—Er—C3	150.25 (8)	H23A—C23—H23C	109.5
C8—Er—C3	80.06 (7)	H23B—C23—H23C	109.5
C6—Er—C3	80.08 (7)	C19—C24—H24A	109.5
C1—Er—C3	59.24 (7)	C19—C24—H24B	109.5
C4—Er—C3	30.80 (7)	H24A—C24—H24B	109.5
C2—Er—C3	30.87 (7)	C19—C24—H24C	109.5
C7—Er—C3	87.93 (7)	H24A—C24—H24C	109.5
C17—N1—C19	108.58 (16)	H24B—C24—H24C	109.5
C17—N1—C25	121.53 (16)	N1—C25—C27	111.65 (16)
C19—N1—C25	129.87 (17)	N1—C25—C26	111.13 (16)
C17—N2—C18	108.34 (16)	C27—C25—C26	113.51 (18)
C17—N2—C20	126.07 (17)	N1—C25—H25	106.7
C18—N2—C20	125.56 (16)	C27—C25—H25	106.7
C8—C1—C2	134.2 (2)	C26—C25—H25	106.7
C8—C1—Er	74.29 (13)	C25—C26—H26A	109.5
C2—C1—Er	74.50 (12)	C25—C26—H26B	109.5
C8—C1—H1	112.9	H26A—C26—H26B	109.5
C2—C1—H1	112.9	C25—C26—H26C	109.5
Er—C1—H1	133.7	H26A—C26—H26C	109.5
C3—C2—C1	135.2 (2)	H26B—C26—H26C	109.5
C3—C2—Er	75.16 (12)	C25—C27—H27A	109.5
C1—C2—Er	74.27 (13)	C25—C27—H27B	109.5
C3—C2—H2	112.4	H27A—C27—H27B	109.5
C1—C2—H2	112.4	C25—C27—H27C	109.5
Er—C2—H2	133.7	H27A—C27—H27C	109.5
C4—C3—C2	135.3 (2)	H27B—C27—H27C	109.5
C4—C3—Er	73.95 (12)		
C8—C1—C2—C3	0.1 (4)	C17—N2—C18—C19	−0.4 (2)
C1—C2—C3—C4	−2.8 (4)	C20—N2—C18—C19	−178.42 (17)
C2—C3—C4—C5	1.4 (4)	C17—N2—C18—C23	179.20 (19)
C3—C4—C5—C6	3.1 (4)	C20—N2—C18—C23	1.2 (3)
C4—C5—C6—C7	−3.2 (4)	N2—C18—C19—N1	0.3 (2)
C5—C6—C7—C8	−1.1 (4)	C23—C18—C19—N1	−179.3 (2)
C2—C1—C8—C7	0.1 (4)	N2—C18—C19—C24	−179.1 (2)
C6—C7—C8—C1	2.4 (4)	C23—C18—C19—C24	1.3 (4)
C16—C9—C10—C11	−1.7 (5)	C17—N1—C19—C18	0.0 (2)
C9—C10—C11—C12	0.3 (5)	C25—N1—C19—C18	178.69 (18)
C10—C11—C12—C13	0.8 (5)	C17—N1—C19—C24	179.4 (2)
C11—C12—C13—C14	−0.4 (5)	C25—N1—C19—C24	−1.9 (3)
C12—C13—C14—C15	0.3 (5)	C17—N2—C20—C21	19.8 (3)
C13—C14—C15—C16	−1.4 (5)	C18—N2—C20—C21	−162.46 (19)
C14—C15—C16—C9	1.2 (5)	C17—N2—C20—C22	−103.6 (2)
C10—C9—C16—C15	0.8 (5)	C18—N2—C20—C22	74.1 (2)

C19—N1—C17—N2	−0.2 (2)	C17—N1—C25—C27	−122.8 (2)
C25—N1—C17—N2	−179.05 (16)	C19—N1—C25—C27	58.6 (3)
C18—N2—C17—N1	0.4 (2)	C17—N1—C25—C26	109.4 (2)
C20—N2—C17—N1	178.39 (17)	C19—N1—C25—C26	−69.2 (3)

C—H···π interactions

D—H···A	Distance H···A (Å)	Angle D—H···A (°)	Symmetry code
C25—H25···*Cg*(C1–C8)	2.27	178	
C17—H17···Cent(C4—C5)	2.33	169	
C20—H20···Cent(C10—C11)	2.58	140	(1/2 + *x*, 0.5 − *y*, 1/2 + *z*)
C22—H22C···Cent(C12—C13)	2.67	151	(1/2 + *x*, 0.5 − *y*, 1/2 + *z*)

Notes: C—H distances are normalized to 1.08 Å, *Cg* is the centre of gravity of a ring and Cent is the mid-point of a bond.

Fig. 1

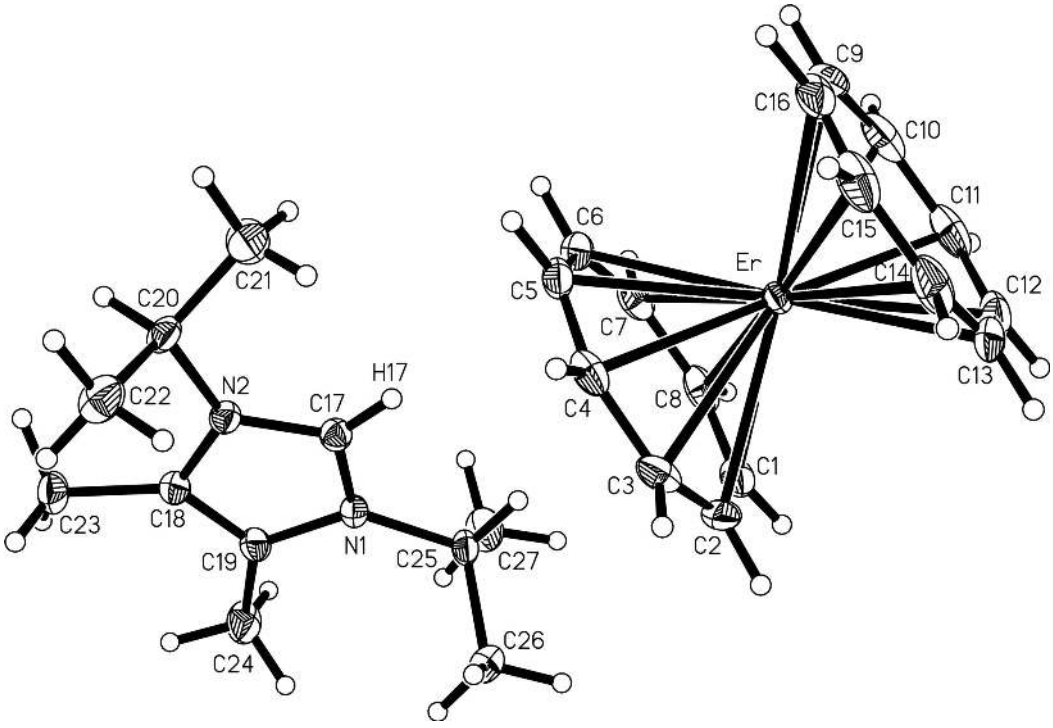
C9
C16
C10
C11
C6
C15
C5
Er
C14
C12
C7
C13
C4
C8
C1
C3
C2
C21
C20
H17
C22
N2
C17
C23
C18
N1
C25
C27
C19
C24
C26

Fig. 2