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An unsolvated erbium organyl: (2,4,6,2″,4″,6″-hexamethyl-1,1′:3′;1″-terphenyl-2′-yl)bis(methylcyclopentadienyl)erbium(III)

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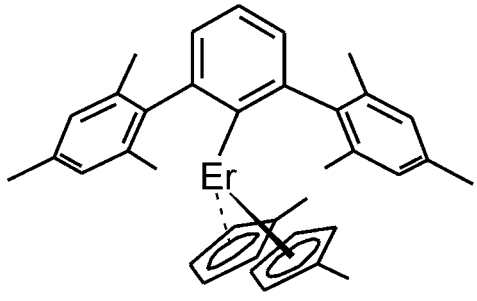
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.007 Å; R factor = 0.040; wR factor = 0.095; data-to-parameter ratio = 21.6.

The title compound, [Er(Dmp)($C_5H_4Me)_2$] (Dmp = 2,6-$Mes_2C_6H_3$, with Mes = 2,4,6-$Me_3C_6H_2$) or [$Er(C_6H_7)_2$-($C_{24}H_{25}$)], was obtained by the reaction of LiDmp with $Er(C_5H_4Me)_3$. The Er atom is η^5-coordinated by two methylcyclopentadienyl ligands (average Er···centroid distance = 2.341 Å) and η^1-coordinated by the *ipso*-C atom of the aryl substituent [Er—C = 2.434 (4) Å]. An additional π-arene contact with one of the Mes groups [Er···C = 3.077 (4) Å] gives rise to the pyramidalization of the metal-atom environment.

Related literature

For other structurally characterized bis(cyclopentadienyl)-lanthanide aryls, see Niemeyer & Hauber(1999). For a review of lanthanide···π-arene interactions, see Bochkarev (2002). For related literature, see: Bochkarev *et al.* (1995); Schumann *et al.* (1995); Tsutsui & Ely (1975).



Experimental

Crystal data

[$Er(C_6H_7)_2(C_{24}H_{25})$]
M_r = 638.93
Monoclinic, $P2_1/c$
a = 9.6758 (9) Å
b = 18.126 (1) Å
c = 16.248 (2) Å
β = 99.428 (7)°
V = 2811.1 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.01 mm^{-1}
T = 173 (2) K
0.50 × 0.30 × 0.25 mm

Data collection

Siemens $P4$ diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.335, T_{max} = 0.504
(expected range = 0.313–0.471)
8124 measured reflections
7465 independent reflections
5572 reflections with $I > 2\sigma(I)$
R_{int} = 0.071
2 standard reflections
every 298 reflections
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.095
S = 1.07
7465 reflections
346 parameters
Only H-atom displacement parameters refined
$\Delta\rho_{max}$ = 1.05 e Å^{-3}
$\Delta\rho_{min}$ = −1.52 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Er—C11	2.434 (4)	Er—C41	2.606 (4)
Er—C31	2.706 (5)	Er—C42	2.620 (4)
Er—C32	2.642 (4)	Er—C43	2.639 (5)
Er—C33	2.591 (4)	Er—C44	2.635 (5)
Er—C34	2.591 (4)	Er—C45	2.623 (4)
Er—C35	2.641 (4)		
C12—C11—Er	108.4 (3)	C16—C11—Er	136.0 (3)

Data collection: *XSCANS* (Siemens, 1994); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2005) and *SHELXTL* (Sheldrick, 1998)'; 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: YA2055).

References

Bochkarev, L. N., Stepantseva, T. A., Zakharov, L. N., Fukin, G. K., Yanovsky, A. I. & Struchkov, Yu. T. (1995). *Organometallics*, **14**, 2127–2129.
Bochkarev, M. N. (2002). *Chem. Rev.* **102**, 2089–2118.
Brandenburg, K. (2005). *DIAMOND*. Version 3.1a. Crystal Impact GbR, Bonn, Germany.
Niemeyer, M. & Hauber, S.-O. (1999). *Z. Anorg. Allg. Chem.* **625**, 137–140.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Schumann, H., Meese-Marktscheffel, J. A. & Esser, L. (1995). *Chem. Rev.* **95**, 865–986.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (1998). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Siemens (1994). *XSCANS*. Release 2.10b. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Tsutsui, M. & Ely, N. M. (1975). *J. Am. Chem. Soc.* **97**, 1280–1281.

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supplementary materials

Acta Cryst. (2007). E**63**, m2188 [**doi:10.1107/S1600536807034575**]

An unsolvated erbium organyl: (2,4,6,2'',4'',6''-hexamethyl-1,1':3';1''-terphenyl-2'-yl)bis(methylcyclopentadienyl)erbium(III)

M. Niemeyer

Comment

Although base-stabilized bis(cyclopentadienyl)lanthanide aryls of the composition ArLnCp'$_2$(thf) (Cp' =Cp, Cp*) have been known for more than three decades and were extensively studied (Tsutsui & Ely, 1975; Schumann *et al.*, 1995), the corresponding Lewis-donor-free systems received much less attention. Earlier we have reported the first structurally characterized examples of this type, which are kinetically stabilized by the bulky Dmp ligand (Niemeyer & Hauber, 1999).

The crystal structure of the title compound, (I), is made up of monomeric units (Fig.1). The erbium atom is coordinated by two η^5-bonded methylcyclopentadienyl ligands (their centroids are X5 and X5') and the *ipso* carbon atom C11 of the Dmp substituent. With 2.434 (4) Å the Er—C11 bond length is practically identical to the average Er—C distance of 2.431 Å in the solvated erbium organyl [Er(Ph)$_3$(thf)$_3$] (Bochkarev *et al.*,1995). The metal-carbon distances to the η^5-coordinated methylcyclopentadienyl rings [average Er–C = 2.629 Å] are typical for other bis(cyclopentadienyl) complexes (Schumann *et al.*, 1995).

The most interesting aspect of the solid-state structure of (I) is additional metal-π-arene interaction (Bochkarev, 2002) involving the Er atom and one of the mesityl rings of the terphenyl substituent, which is reflected in dramatically different Er···C21 and Er···C61 distances [Er···C21 = 3.077 (4) Å; Er···C61 = 3.945 (4) Å] as well as quite different Er—C11—C12 and Er—C11—C16 angles [136.0 (3)° and 108.4 (3)° respectively]. This interaction also causes a noticeable pyramidalization of the metal coordination: taking the centroids of the methylcyclopentadienyl rings and C11 as a reference, the sum of the angles around Er is calculated to be 353.6°. Alternatively, the degree of pyramidalization may be characterized by the displacement of the metal atom from the least-squares plane defined by X5, X5' and C11, which amounts to 0.348 (4) Å.

Experimental

A solution of LiDmp (0.81 g, 2.54 mmol) and Er(C$_5$H$_4$Me)$_3$ (1.03 g, 2.54 mmol) in 20 ml of toluene was stirred for 14 h under an atmosphere of purified argon, after which all volatile materials were removed under reduced pressure. The remaining solid was extracted with a 1:4 mixture of toluene and *n*-heptane (*ca* 15 ml) and solid by-products were separated by filtration. Storage of the resulting pink solution in a 248 K freezer overnight afforded pale pink crystals of (I) (yield 61%), which were suitable for X-ray study.

m.p. 427–428 K (dec); EI—MS (70 eV, 420 K): m/*z* (%) 314.2 (100) [Dmp$^+$], 324.0 (13) [{Er(C$_5$H$_4$Me)$_2$}$^+$], 558.2 (4.1)[{DmpErC$_5$H$_4$Me}$^+$], 639.2 (2.6) [*M*$^+$]. Anal. Calcd for C$_{36}$H$_{39}$Er: C, 67.67; H, 6.15. Found: C, 67.65; H, 6.30.

Refinement

The H atoms were positioned geometrically at distances of 0.95 (Aryl-H), 0.98 (CH_3) and 1.00 Å (MeC_5H_3—H) and refined in a riding model approximation, including free rotation for methyl groups. A common isotropic displacement parameter was refined for H atoms belonging to the CH (aryl), CH (C_5H_4Me) CH_3 (Mes) and CH_3 (C_5H_4Me) groups. The highest residual density of 1.05 e A°$^{-3}$ and the deepest hole of −1.52 e A°$^{-3}$ are located near the Er atom.

Figures

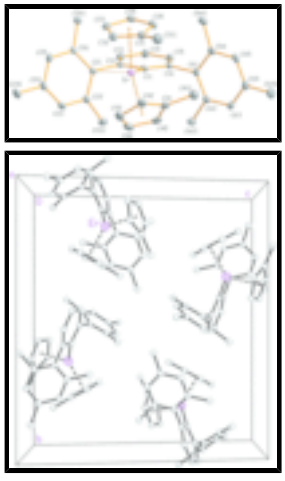


Fig. 1. The molecular structure of (I), with atom labels and 30% probability displacement ellipsoids. H atoms have been omitted.

(2,4,6,2'',4'',6''-hexamethyl-1,1':3',1''-terphenyl-2'-yl)\ bis(methylcyclopentadienyl)erbium(III)

Crystal data

$[Er(C_6H_7)_2(C_{24}H_{25})]$	F_{000} = 1292
M_r = 638.93	D_x = 1.510 Mg m^{-3}
Monoclinic, $P2_1/c$	Melting point: 428 K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation λ = 0.71069 Å
a = 9.6758 (9) Å	Cell parameters from 48 reflections
b = 18.126 (1) Å	θ = 6.0–12.5º
c = 16.248 (2) Å	μ = 3.01 mm^{-1}
β = 99.428 (7)º	T = 173 (2) K
V = 2811.1 (5) Å^3	Prism, pale pink
Z = 4	0.50 × 0.30 × 0.25 mm

Data collection

Siemens P4 diffractometer	R_{int} = 0.071
Radiation source: fine-focus sealed tube	θ_{max} = 29.0º
Monochromator: graphite	θ_{min} = 2.1º

T = 173(2) K
ω scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.335, T_{max} = 0.504
8124 measured reflections
7465 independent reflections
5572 reflections with $I > 2\sigma(I)$

$h = -13 \rightarrow 13$
$k = 0 \rightarrow 24$
$l = 0 \rightarrow 22$
2 standard reflections
every 298 reflections
intensity decay: none

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.095$
S = 1.07
7465 reflections
346 parameters
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
Only H-atom displacement parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0351P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.05$ e Å^{-3}
$\Delta\rho_{min} = -1.52$ 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	0.78480 (2)	0.160221 (10)	0.337742 (12)	0.02371 (6)
C11	0.5701 (4)	0.0878 (2)	0.3177 (3)	0.0220 (8)
C12	0.5970 (4)	0.0191 (2)	0.2803 (2)	0.0203 (7)
C13	0.5040 (5)	−0.0397 (2)	0.2735 (3)	0.0272 (9)
H13A	0.5275	−0.0848	0.2494	0.034 (5)*
C14	0.3776 (5)	−0.0330 (2)	0.3016 (3)	0.0281 (9)
H14A	0.3141	−0.0733	0.2975	0.034 (5)*
C15	0.3442 (5)	0.0339 (2)	0.3362 (3)	0.0266 (9)
H15A	0.2569	0.0393	0.3551	0.034 (5)*
C16	0.4383 (4)	0.0931 (2)	0.3432 (2)	0.0207 (8)

C21	0.7283 (4)	0.0143 (2)	0.2413 (2)	0.0211 (8)
C22	0.7303 (5)	0.0528 (2)	0.1659 (3)	0.0260 (9)
C23	0.8529 (5)	0.0517 (2)	0.1304 (3)	0.0304 (10)
H23A	0.8558	0.0793	0.0810	0.034 (5)*
C24	0.9699 (5)	0.0117 (2)	0.1648 (3)	0.0277 (9)
C25	0.9613 (4)	−0.0306 (2)	0.2358 (3)	0.0260 (9)
H25A	1.0391	−0.0601	0.2589	0.034 (5)*
C26	0.8426 (5)	−0.0307 (2)	0.2736 (2)	0.0234 (8)
C31	0.9460 (5)	0.1945 (3)	0.4850 (3)	0.0296 (9)
C32	1.0263 (5)	0.1502 (2)	0.4400 (3)	0.0291 (9)
H32A	1.1198	0.1637	0.4258	0.045 (6)*
C33	0.9663 (5)	0.0792 (3)	0.4322 (3)	0.0307 (10)
H33A	1.0121	0.0340	0.4140	0.045 (6)*
C34	0.8454 (5)	0.0800 (3)	0.4707 (3)	0.0297 (9)
H34A	0.7922	0.0354	0.4840	0.045 (6)*
C35	0.8312 (5)	0.1508 (3)	0.5022 (3)	0.0302 (9)
H35A	0.7636	0.1654	0.5397	0.045 (6)*
C41	0.7264 (6)	0.3005 (2)	0.3245 (3)	0.0317 (10)
C42	0.8693 (5)	0.2952 (2)	0.3166 (3)	0.0316 (10)
H42A	0.9480	0.3207	0.3533	0.045 (6)*
C43	0.8798 (6)	0.2591 (3)	0.2417 (3)	0.0378 (11)
H43A	0.9668	0.2544	0.2164	0.045 (6)*
C44	0.7445 (6)	0.2425 (3)	0.2023 (3)	0.0397 (12)
H44A	0.7193	0.2234	0.1440	0.045 (6)*
C45	0.6479 (5)	0.2677 (3)	0.2522 (3)	0.0358 (11)
H45A	0.5440	0.2708	0.2349	0.045 (6)*
C61	0.3927 (4)	0.1652 (2)	0.3759 (2)	0.0220 (7)
C62	0.3219 (5)	0.2171 (2)	0.3206 (3)	0.0257 (9)
C63	0.2844 (5)	0.2850 (2)	0.3510 (3)	0.0280 (9)
H63A	0.2375	0.3202	0.3130	0.034 (5)*
C64	0.3137 (5)	0.3025 (3)	0.4350 (3)	0.0301 (9)
C65	0.3779 (5)	0.2494 (3)	0.4898 (3)	0.0291 (9)
H65A	0.3959	0.2603	0.5478	0.034 (5)*
C66	0.4170 (4)	0.1805 (2)	0.4627 (3)	0.0251 (9)
C221	0.5983 (5)	0.0849 (3)	0.1176 (3)	0.0344 (10)
H22A	0.6203	0.1111	0.0685	0.064 (5)*
H22B	0.5571	0.1195	0.1531	0.064 (5)*
H22C	0.5315	0.0452	0.0996	0.064 (5)*
C241	1.0993 (5)	0.0103 (3)	0.1238 (3)	0.0390 (11)
H24A	1.1133	0.0590	0.1004	0.064 (5)*
H24B	1.0874	−0.0266	0.0791	0.064 (5)*
H24C	1.1811	−0.0025	0.1654	0.064 (5)*
C261	0.8379 (5)	−0.0808 (2)	0.3474 (3)	0.0291 (9)
H26A	0.9334	−0.0953	0.3718	0.064 (5)*
H26B	0.7829	−0.1249	0.3289	0.064 (5)*
H26C	0.7942	−0.0546	0.3893	0.064 (5)*
C311	0.9865 (7)	0.2687 (3)	0.5224 (4)	0.0454 (13)
H31A	1.0307	0.2625	0.5807	0.144 (17)*
H31B	0.9026	0.2995	0.5198	0.144 (17)*

H31C	1.0526	0.2925	0.4911	0.144 (17)*
C411	0.6647 (6)	0.3360 (3)	0.3947 (4)	0.0454 (12)
H41A	0.6583	0.3894	0.3860	0.144 (17)*
H41B	0.7249	0.3256	0.4481	0.144 (17)*
H41C	0.5709	0.3159	0.3956	0.144 (17)*
C621	0.2827 (6)	0.1990 (3)	0.2291 (3)	0.0356 (11)
H62A	0.2570	0.2445	0.1976	0.064 (5)*
H62B	0.2030	0.1649	0.2210	0.064 (5)*
H62C	0.3627	0.1760	0.2091	0.064 (5)*
C641	0.2815 (6)	0.3791 (3)	0.4654 (3)	0.0434 (13)
H64A	0.1865	0.3935	0.4398	0.064 (5)*
H64B	0.3490	0.4146	0.4498	0.064 (5)*
H64C	0.2881	0.3784	0.5263	0.064 (5)*
C661	0.4763 (5)	0.1222 (3)	0.5246 (3)	0.0349 (10)
H66A	0.5096	0.1453	0.5788	0.064 (5)*
H66B	0.5545	0.0973	0.5048	0.064 (5)*
H66C	0.4032	0.0861	0.5306	0.064 (5)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Er	0.02356 (9)	0.02370 (9)	0.02381 (9)	−0.00197 (9)	0.00372 (6)	0.00470 (8)
C11	0.024 (2)	0.0229 (18)	0.0203 (19)	−0.0004 (16)	0.0064 (16)	0.0027 (15)
C12	0.0199 (18)	0.0242 (18)	0.0165 (17)	0.0038 (15)	0.0024 (14)	0.0027 (15)
C13	0.029 (2)	0.024 (2)	0.028 (2)	0.0015 (17)	0.0027 (18)	0.0004 (16)
C14	0.024 (2)	0.026 (2)	0.035 (2)	−0.0014 (17)	0.0031 (18)	0.0007 (17)
C15	0.0185 (19)	0.029 (2)	0.033 (2)	−0.0001 (17)	0.0067 (17)	0.0016 (17)
C16	0.0192 (18)	0.0269 (19)	0.0162 (17)	0.0022 (15)	0.0034 (15)	0.0028 (15)
C21	0.0239 (19)	0.0208 (17)	0.0191 (18)	0.0002 (15)	0.0047 (15)	−0.0009 (15)
C22	0.029 (2)	0.0266 (19)	0.0231 (19)	0.0033 (17)	0.0057 (17)	0.0013 (17)
C23	0.040 (3)	0.029 (2)	0.024 (2)	0.0041 (19)	0.0121 (19)	0.0057 (17)
C24	0.026 (2)	0.030 (2)	0.030 (2)	−0.0007 (18)	0.0121 (18)	−0.0058 (18)
C25	0.0197 (19)	0.028 (2)	0.031 (2)	0.0051 (16)	0.0049 (17)	−0.0051 (17)
C26	0.029 (2)	0.025 (2)	0.0170 (18)	0.0031 (17)	0.0075 (16)	−0.0025 (15)
C31	0.030 (2)	0.030 (2)	0.028 (2)	−0.0001 (19)	0.0023 (18)	0.0002 (18)
C32	0.0214 (19)	0.036 (2)	0.028 (2)	−0.0030 (18)	0.0008 (16)	−0.0011 (18)
C33	0.033 (2)	0.030 (2)	0.027 (2)	0.0061 (19)	−0.0002 (19)	0.0020 (18)
C34	0.031 (2)	0.032 (2)	0.025 (2)	−0.0036 (18)	0.0003 (18)	0.0075 (18)
C35	0.026 (2)	0.040 (3)	0.025 (2)	−0.0020 (19)	0.0072 (17)	0.0000 (18)
C41	0.042 (3)	0.021 (2)	0.033 (2)	0.0034 (19)	0.009 (2)	0.0077 (17)
C42	0.034 (2)	0.026 (2)	0.035 (2)	−0.0040 (19)	0.009 (2)	0.0056 (18)
C43	0.044 (3)	0.034 (2)	0.040 (3)	−0.002 (2)	0.021 (2)	0.006 (2)
C44	0.055 (3)	0.039 (3)	0.026 (2)	−0.003 (2)	0.008 (2)	0.006 (2)
C45	0.037 (3)	0.030 (2)	0.040 (3)	0.002 (2)	0.003 (2)	0.018 (2)
C61	0.0174 (17)	0.0259 (19)	0.0238 (18)	0.0000 (16)	0.0067 (14)	−0.0015 (16)
C62	0.028 (2)	0.028 (2)	0.022 (2)	0.0033 (17)	0.0074 (16)	−0.0003 (16)
C63	0.027 (2)	0.027 (2)	0.030 (2)	0.0081 (18)	0.0054 (19)	0.0019 (17)
C64	0.027 (2)	0.032 (2)	0.032 (2)	0.0030 (18)	0.0086 (19)	−0.0054 (19)

C65	0.026 (2)	0.038 (2)	0.025 (2)	0.0007 (19)	0.0102 (18)	−0.0052 (18)
C66	0.0171 (18)	0.035 (2)	0.024 (2)	−0.0003 (16)	0.0060 (16)	0.0032 (16)
C221	0.037 (3)	0.037 (2)	0.028 (2)	0.009 (2)	0.001 (2)	0.0080 (19)
C241	0.040 (3)	0.047 (3)	0.035 (3)	0.000 (2)	0.019 (2)	0.000 (2)
C261	0.035 (2)	0.029 (2)	0.024 (2)	0.0021 (19)	0.0050 (18)	0.0021 (17)
C311	0.053 (3)	0.039 (3)	0.045 (3)	−0.002 (3)	0.007 (3)	−0.006 (2)
C411	0.052 (3)	0.044 (3)	0.042 (3)	0.008 (3)	0.014 (2)	0.001 (2)
C621	0.045 (3)	0.039 (3)	0.022 (2)	0.008 (2)	0.001 (2)	0.0015 (19)
C641	0.050 (3)	0.039 (3)	0.042 (3)	0.006 (2)	0.010 (3)	−0.012 (2)
C661	0.035 (3)	0.047 (3)	0.024 (2)	−0.001 (2)	0.0079 (19)	0.005 (2)

Geometric parameters (Å, °)

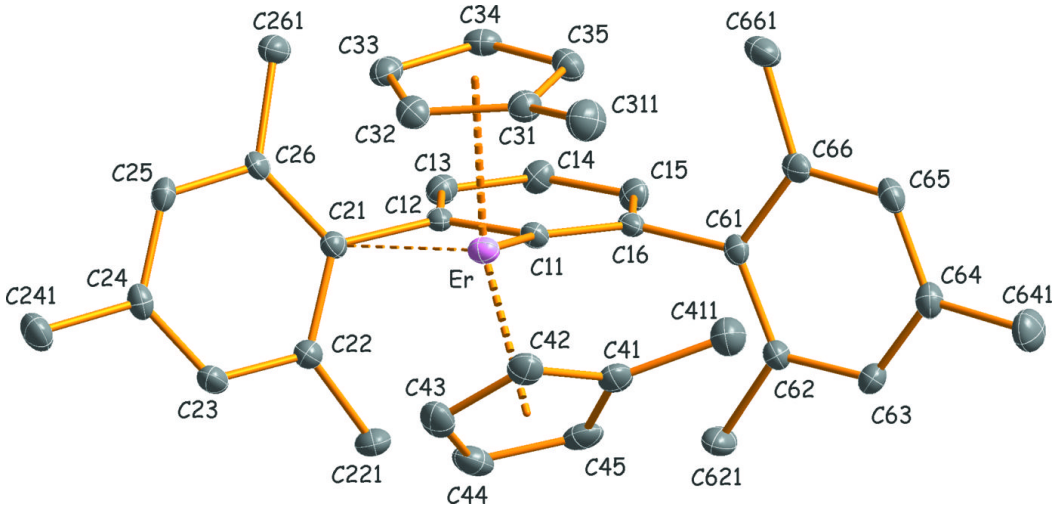
Er—C11	2.434 (4)	C41—C45	1.420 (7)
Er—C31	2.706 (5)	C41—C411	1.516 (7)
Er—C32	2.642 (4)	C42—C43	1.400 (7)
Er—C33	2.591 (4)	C42—H42A	1.0000
Er—C34	2.591 (4)	C43—C44	1.393 (8)
Er—C35	2.641 (4)	C43—H43A	1.0000
Er—C41	2.606 (4)	C44—C45	1.410 (7)
Er—C42	2.620 (4)	C44—H44A	1.0000
Er—C43	2.639 (5)	C45—H45A	1.0000
Er—C44	2.635 (5)	C61—C62	1.400 (6)
Er—C45	2.623 (4)	C61—C66	1.419 (6)
C11—C16	1.407 (6)	C62—C63	1.398 (6)
C11—C12	1.427 (5)	C62—C621	1.509 (6)
C12—C13	1.388 (6)	C63—C64	1.384 (6)
C12—C21	1.512 (5)	C63—H63A	0.9500
C13—C14	1.379 (6)	C64—C65	1.387 (7)
C13—H13A	0.9500	C64—C641	1.523 (7)
C14—C15	1.396 (6)	C65—C66	1.397 (6)
C14—H14A	0.9500	C65—H65A	0.9500
C15—C16	1.399 (6)	C66—C661	1.506 (6)
C15—H15A	0.9500	C221—H22A	0.9800
C16—C61	1.505 (6)	C221—H22B	0.9800
C21—C26	1.406 (6)	C221—H22C	0.9800
C21—C22	1.413 (6)	C241—H24A	0.9800
C22—C23	1.402 (6)	C241—H24B	0.9800
C22—C221	1.502 (6)	C241—H24C	0.9800
C23—C24	1.383 (6)	C261—H26A	0.9800
C23—H23A	0.9500	C261—H26B	0.9800
C24—C25	1.398 (6)	C261—H26C	0.9800
C24—C241	1.512 (6)	C311—H31A	0.9800
C25—C26	1.388 (6)	C311—H31B	0.9800
C25—H25A	0.9500	C311—H31C	0.9800
C26—C261	1.509 (6)	C411—H41A	0.9800
C31—C32	1.403 (6)	C411—H41B	0.9800
C31—C35	1.429 (6)	C411—H41C	0.9800
C31—C311	1.501 (7)	C621—H62A	0.9800

C32—C33	1.409 (6)	C621—H62B	0.9800
C32—H32A	1.0000	C621—H62C	0.9800
C33—C34	1.414 (7)	C641—H64A	0.9800
C33—H33A	1.0000	C641—H64B	0.9800
C34—C35	1.396 (6)	C641—H64C	0.9800
C34—H34A	1.0000	C661—H66A	0.9800
C35—H35A	1.0000	C661—H66B	0.9800
C41—C42	1.412 (7)	C661—H66C	0.9800
C11—Er—C34	83.11 (14)	C35—C34—C33	108.0 (4)
C11—Er—C33	104.71 (14)	C35—C34—Er	76.5 (3)
C34—Er—C33	31.67 (15)	C33—C34—Er	74.2 (2)
C11—Er—C41	110.29 (15)	C35—C34—H34A	125.4
C34—Er—C41	129.28 (15)	C33—C34—H34A	125.4
C33—Er—C41	135.95 (16)	Er—C34—H34A	125.4
C11—Er—C42	139.83 (14)	C34—C35—C31	108.2 (4)
C34—Er—C42	126.92 (15)	C34—C35—Er	72.5 (3)
C33—Er—C42	114.29 (15)	C31—C35—Er	77.0 (3)
C41—Er—C42	31.35 (15)	C34—C35—H35A	125.4
C11—Er—C45	89.10 (15)	C31—C35—H35A	125.4
C34—Er—C45	152.19 (16)	Er—C35—H35A	125.4
C33—Er—C45	165.78 (16)	C42—C41—C45	107.2 (4)
C41—Er—C45	31.51 (15)	C42—C41—C411	127.5 (5)
C42—Er—C45	51.54 (16)	C45—C41—C411	125.2 (5)
C11—Er—C44	100.81 (15)	C42—C41—Er	74.9 (3)
C34—Er—C44	175.50 (16)	C45—C41—Er	74.9 (3)
C33—Er—C44	144.02 (16)	C411—C41—Er	117.3 (3)
C41—Er—C44	51.54 (16)	C43—C42—C41	108.8 (5)
C42—Er—C44	50.84 (16)	C43—C42—Er	75.3 (3)
C45—Er—C44	31.11 (16)	C41—C42—Er	73.8 (3)
C11—Er—C43	131.29 (16)	C43—C42—H42A	125.2
C34—Er—C43	145.23 (16)	C41—C42—H42A	125.2
C33—Er—C43	117.89 (17)	Er—C42—H42A	125.2
C41—Er—C43	51.68 (15)	C44—C43—C42	107.7 (5)
C42—Er—C43	30.87 (15)	C44—C43—Er	74.5 (3)
C45—Er—C43	51.42 (16)	C42—C43—Er	73.8 (3)
C44—Er—C43	30.63 (17)	C44—C43—H43A	125.7
C11—Er—C35	95.75 (14)	C42—C43—H43A	125.7
C34—Er—C35	30.93 (14)	Er—C43—H43A	125.7
C33—Er—C35	51.49 (15)	C43—C44—C45	109.1 (5)
C41—Er—C35	98.37 (15)	C43—C44—Er	74.9 (3)
C42—Er—C35	100.84 (15)	C45—C44—Er	74.0 (3)
C45—Er—C35	124.86 (16)	C43—C44—H44A	125.1
C44—Er—C35	149.23 (16)	C45—C44—H44A	125.1
C43—Er—C35	128.62 (16)	Er—C44—H44A	125.1
C11—Er—C32	133.97 (14)	C44—C45—C41	107.2 (5)
C34—Er—C32	51.76 (14)	C44—C45—Er	74.9 (3)
C33—Er—C32	31.22 (14)	C41—C45—Er	73.6 (3)
C41—Er—C32	106.06 (15)	C44—C45—H45A	125.9
C42—Er—C32	83.34 (15)	C41—C45—H45A	125.9

C45—Er—C32	134.59 (15)	Er—C45—H45A	125.9
C44—Er—C32	123.99 (16)	C62—C61—C66	119.4 (4)
C43—Er—C32	93.49 (16)	C62—C61—C16	119.8 (4)
C35—Er—C32	51.18 (14)	C66—C61—C16	120.7 (4)
C11—Er—C31	126.72 (14)	C63—C62—C61	119.5 (4)
C34—Er—C31	51.14 (14)	C63—C62—C621	120.1 (4)
C33—Er—C31	50.93 (14)	C61—C62—C621	120.4 (4)
C41—Er—C31	86.26 (15)	C64—C63—C62	121.8 (4)
C42—Er—C31	75.78 (15)	C64—C63—H63A	119.1
C45—Er—C31	117.76 (15)	C62—C63—H63A	119.1
C44—Er—C31	126.43 (16)	C63—C64—C65	118.2 (4)
C43—Er—C31	99.25 (16)	C63—C64—C641	120.5 (4)
C35—Er—C31	30.97 (14)	C65—C64—C641	121.2 (4)
C32—Er—C31	30.40 (14)	C64—C65—C66	122.2 (4)
C16—C11—C12	114.9 (4)	C64—C65—H65A	118.9
C12—C11—Er	108.4 (3)	C66—C65—H65A	118.9
C16—C11—Er	136.0 (3)	C65—C66—C61	118.6 (4)
C13—C12—C11	122.9 (4)	C65—C66—C661	120.6 (4)
C13—C12—C21	120.0 (4)	C61—C66—C661	120.7 (4)
C11—C12—C21	116.9 (4)	C22—C221—H22A	109.5
C14—C13—C12	120.2 (4)	C22—C221—H22B	109.5
C14—C13—H13A	119.9	H22A—C221—H22B	109.5
C12—C13—H13A	119.9	C22—C221—H22C	109.5
C13—C14—C15	119.1 (4)	H22A—C221—H22C	109.5
C13—C14—H14A	120.4	H22B—C221—H22C	109.5
C15—C14—H14A	120.4	C24—C241—H24A	109.5
C14—C15—C16	120.5 (4)	C24—C241—H24B	109.5
C14—C15—H15A	119.8	H24A—C241—H24B	109.5
C16—C15—H15A	119.8	C24—C241—H24C	109.5
C15—C16—C11	122.2 (4)	H24A—C241—H24C	109.5
C15—C16—C61	118.0 (4)	H24B—C241—H24C	109.5
C11—C16—C61	119.7 (4)	C26—C261—H26A	109.5
C26—C21—C22	119.3 (4)	C26—C261—H26B	109.5
C26—C21—C12	122.7 (3)	H26A—C261—H26B	109.5
C22—C21—C12	117.8 (4)	C26—C261—H26C	109.5
C23—C22—C21	118.8 (4)	H26A—C261—H26C	109.5
C23—C22—C221	119.7 (4)	H26B—C261—H26C	109.5
C21—C22—C221	120.9 (4)	C31—C311—H31A	109.5
C24—C23—C22	122.2 (4)	C31—C311—H31B	109.5
C24—C23—H23A	118.9	H31A—C311—H31B	109.5
C22—C23—H23A	118.9	C31—C311—H31C	109.5
C23—C24—C25	117.8 (4)	H31A—C311—H31C	109.5
C23—C24—C241	120.8 (4)	H31B—C311—H31C	109.5
C25—C24—C241	121.3 (4)	C41—C411—H41A	109.5
C26—C25—C24	122.1 (4)	C41—C411—H41B	109.5
C26—C25—H25A	118.9	H41A—C411—H41B	109.5
C24—C25—H25A	118.9	C41—C411—H41C	109.5
C25—C26—C21	119.4 (4)	H41A—C411—H41C	109.5
C25—C26—C261	119.2 (4)	H41B—C411—H41C	109.5

C21—C26—C261	121.4 (4)	C62—C621—H62A	109.5
C32—C31—C35	107.4 (4)	C62—C621—H62B	109.5
C32—C31—C311	126.4 (5)	H62A—C621—H62B	109.5
C35—C31—C311	125.3 (4)	C62—C621—H62C	109.5
C32—C31—Er	72.3 (3)	H62A—C621—H62C	109.5
C35—C31—Er	72.0 (3)	H62B—C621—H62C	109.5
C311—C31—Er	129.7 (3)	C64—C641—H64A	109.5
C31—C32—C33	108.3 (4)	C64—C641—H64B	109.5
C31—C32—Er	77.3 (3)	H64A—C641—H64B	109.5
C33—C32—Er	72.4 (3)	C64—C641—H64C	109.5
C31—C32—H32A	125.3	H64A—C641—H64C	109.5
C33—C32—H32A	125.3	H64B—C641—H64C	109.5
Er—C32—H32A	125.3	C66—C661—H66A	109.5
C32—C33—C34	108.1 (4)	C66—C661—H66B	109.5
C32—C33—Er	76.4 (3)	H66A—C661—H66B	109.5
C34—C33—Er	74.2 (3)	C66—C661—H66C	109.5
C32—C33—H33A	125.4	H66A—C661—H66C	109.5
C34—C33—H33A	125.4	H66B—C661—H66C	109.5
Er—C33—H33A	125.4		

Fig. 1


C261
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C621
C44

Fig. 2