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(η^8-Cyclooctatetraenyl)(*m*-terphenyl)yttrium-μ-chloro-[tris(tetrahydrofuran)lithium(I)]

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The molecular structure of a mixed terphenyl COT complex [COT is cyclooctatetraene] of the element yttrium of composition (Dpp)Y(COT)(μ-Cl)Li(THF)$_3$ [Dpp is 2,6-diphenylphenyl and THF is tetrahydrofuran] or [LiY(C_8H_8)($C_{18}H_{13}$)Cl(C_4H_8O)] is reported. The monomeric complex is composed of one η^8-bonded COT and one σ-bonded terphenyl ligand, as well as a lithium chloride moiety with the alkali metal atom being solvated by three tetrahydrofuran molecules.

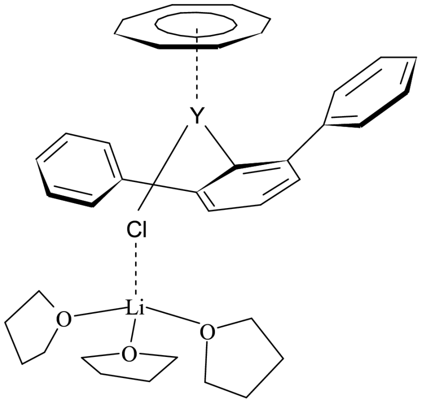
Key indicators

Single-crystal X-ray study
T = 218 K
Mean σ(C–C) = 0.008 Å
Disorder in main residue
R factor = 0.038
wR factor = 0.070
Data-to-parameter ratio = 12.3

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

We were interested in investigating the accessibility of mixed terphenyl COT compounds of the lanthanides and their congeners. Our previous studies have shown that such compounds are, in principle, accessible for the lanthanide elements samarium (Rabe *et al.*, 2003) and lutetium (Rabe *et al.*, 2004) in a one-pot synthesis.



(I)

The average Y—C$_{COT}$ distance in the title compound, (I), is 2.564 Å, while the Y—centroid distance is 1.80 (4) Å, with centroid—Y—Cl1 and centroid—Y—C9 angles of 129.1 (4) and 135.3 (4) °, respectively. In addition to the Y—C9 distance of 2.463 (4) Å the next closest Y—terphenyl distances are to C atoms C16 [3.317 (4) Å] and C22 [3.229 (4) Å], indicating possible weak allyl-like interactions. The dihedral angles between the central (C9–C14) and outer aryl rings (C15–C20 and C21–C26) are both 41.2 (1)°. (I) is isostructural with its samarium and lutetium analogs (Rabe *et al.*, 2003; Rabe *et al.*, 2004).

Experimental

Single crystalline material of (I) was obtained from the one-pot reaction of equimolar amounts of K$_2$COT (Katz, 1960), YCl$_3$ and

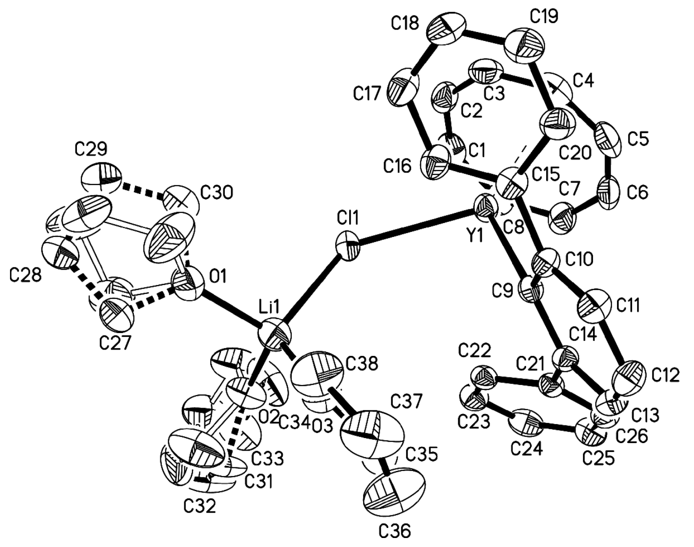


Figure 1
The molecular structure of the title compound, showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms have been omitted for clarity. Heavy dashed and open lines are used to highlight the disorder with respect to C atoms of the THF groups. For clarity, only one set of C atoms of each disordered THF ring is labeled.

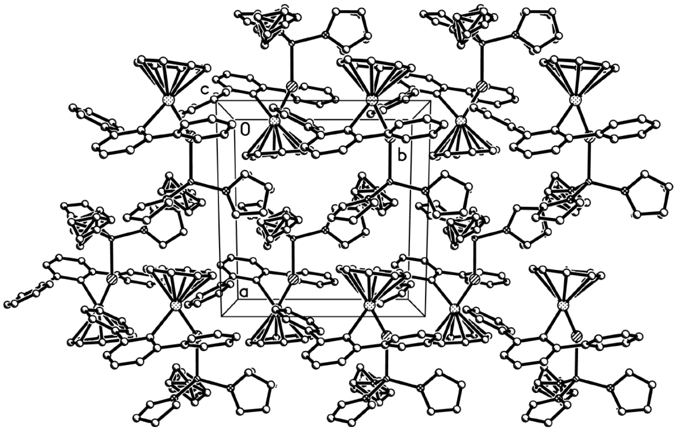


Figure 2
Unit cell contents, viewed along the *c* axis. All H atoms have been omitted for clarity.

DppLi (Rabe *et al.*, 2000) in tetrahydrofuran (THF) at room temperature, followed by extraction of the crude product with toluene in the presence of a couple of drops of THF and cooling to 248 K.

Crystal data

$[LiY(C_8H_8)(C_{18}H_{13})Cl(C_4H_8O)_3]$
$M_r = 681.04$
Monoclinic, $P2_1$
$a = 11.520\ (3)$ Å
$b = 10.420\ (3)$ Å
$c = 16.011\ (5)$ Å
$\beta = 111.084\ (5)°$
$V = 1793.1\ (9)$ Å^3
$Z = 2$

$D_x = 1.261$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 500 reflections
$\theta = 2.5$–$25.0°$
$\mu = 1.73$ mm^{-1}
$T = 218\ (2)$ K
Block, colorless
0.20 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min} = 0.709$, $T_{max} = 0.709$
11 229 measured reflections

5812 independent reflections
4012 reflections with $I > 2\sigma(I)$
$R_{int} = 0.046$
$\theta_{max} = 25.5°$
$h = -12 \rightarrow 13$
$k = -12 \rightarrow 12$
$l = -17 \rightarrow 19$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.070$
$S = 0.85$
5812 reflections
471 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.005P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.029$
$\Delta\rho_{max} = 0.43$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ e Å^{-3}
Absolute structure: Flack (1983), 2280 Friedel pairs
Flack parameter = 0.010 (6)

Table 1
Selected geometric parameters (Å, °) for (I).

Y1—C9	2.463 (4)	Y1—C5	2.573 (6)
Y1—C7	2.537 (6)	Y1—C2	2.593 (5)
Y1—C4	2.530 (5)	Y1—C1	2.616 (5)
Y1—C6	2.546 (4)	Y1—Cl1	2.6688 (13)
Y1—C3	2.551 (5)	Cl1—Li1	2.357 (8)
Y1—C8	2.565 (5)		
C9—Y1—Cl1	95.47 (10)	C10—C9—Y1	122.2 (3)
Li1—Cl1—Y1	135.8 (2)	C14—C9—Y1	120.9 (3)

Atoms C27—C30 and C31—C34 of the THF rings were found to be disordered over two positions, with percent occupancies of 66 (1)/34 (1) and 44 (2)/56 (2), respectively. The disordered THF groups were refined with restraints on geometry and displacement parameters. Even though the disorder was modeled, some C atoms, especially C30 and C30A, of the THF rings still showed large displacement parameters. All H atoms were placed in calculated positions (C—H = 0.94–0.98 Å), with isotropic displacement parameters fixed at 1.2 or 1.5 times U_{eq} of the parent atom, and were refined as riding atoms.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SMART*; data reduction: *SAINT* and *SHELXTL* (Bruker, 2001); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Acta Cryst. (2004). E**60**, m1442–m1443 Gerd W. Rabe *et al.* • $[LiY(C_8H_8)(C_{18}H_{13})Cl(C_4H_8O)_3]$ **m1443**