

# Bis[ $\mu$ - $\eta^5$ : $\eta^1$ -2-(cyclopentadienyl)ethoxy]-bis[( $\eta^5$ -cyclopentadienyl)(1,2-dimethoxyethane- $\kappa$ O)yttrium]

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## Key indicators

Single-crystal X-ray study

$T = 173$  K

Mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å

$R$  factor = 0.045

$wR$  factor = 0.088

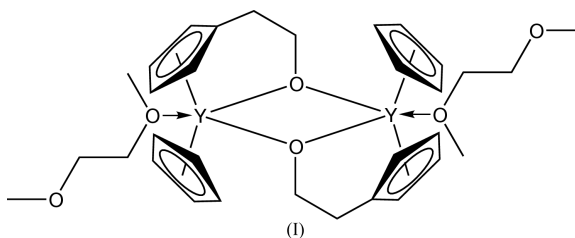
Data-to-parameter ratio = 19.0

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

The reaction of  $\text{Cp}_3\text{Y}$  with 2,4-cyclopentadiene-1-ethanol and recrystallization from 1,2-dimethoxyethane (dme) gave the title compound,  $[\text{CpY}(\mu\text{-}\eta^5\text{:}\eta^1\text{-C}_5\text{H}_4\text{CH}_2\text{CH}_2\text{O})(\text{dme})]_2$  or  $[\text{Y}_2(\text{C}_5\text{H}_5)_2(\text{C}_7\text{H}_8\text{O})_2(\text{C}_4\text{H}_{10}\text{O}_2)_2]$ . Bond lengths and angles of the dimeric complex are comparable with similar cyclopentadienyl and  $\mu$ -alkoxo complexes of yttrium. The complex has crystallographically imposed inversion symmetry and features two Y atoms that exist in distorted trigonal bipyramidal coordination geometries.

## Comment

The title compound, (I), possesses crystallographically imposed inversion symmetry. Both Y atoms of the dimeric complex are bridged by the two O atoms of the 2-(cyclopentadienyl)ethoxy ligands. The metal centers are coordinated to two cyclopentadienyl rings and three O atoms, by two cyclopentadienylethoxide O atoms and one O atom of the dme ligand. The coordination geometry around each Y atom corresponds to a distorted trigonal bipyramid. The distances of the metal centers to the bridging O atoms are longer than those reported for the dimeric alkoxides  $[(\text{Me}_3\text{SiC}_5\text{H}_4)_2\text{Y}(\mu\text{-OMe})]_2$  [2.217 (3) and 2.233 (3) Å; Evans *et al.*, 1992] and  $[(\text{MeC}_5\text{H}_4)_2\text{Y}(\mu\text{-O}^i\text{Pr})]_2$  [2.2228 (19) and 2.2432 (19) Å; Li *et al.*, 2000], but comparable with the values found in  $[(\text{MeC}_5\text{H}_4)_2\text{Y}(\mu\text{-OCH}=\text{CH}_2)]_2$  [2.275 (3) and 2.290 (3) Å; Evans *et al.*, 1986].



Only one O atom of the bidentate 1,2-dimethoxyethane (dme) ligand is coordinated to the metal center. Compared to the Y–O bond lengths of the alkoxide O atoms, the distance between the metal center and the dme O atom is much longer. A similar value was observed for the Y–O distance to THF in  $\text{Cp}_3\text{Y}(\text{THF})$  [2.451 (4) Å; Rogers *et al.*, 1981]. A shorter distance was reported for the alkoxide  $(\text{Cp}^*\text{Y})_2(\mu\text{-OCH}_2\text{CH}_2\text{O})(\text{THF})_2$  [Y–O<sub>THF</sub> 2.398 (5) Å; Deelman *et al.*, 1995].

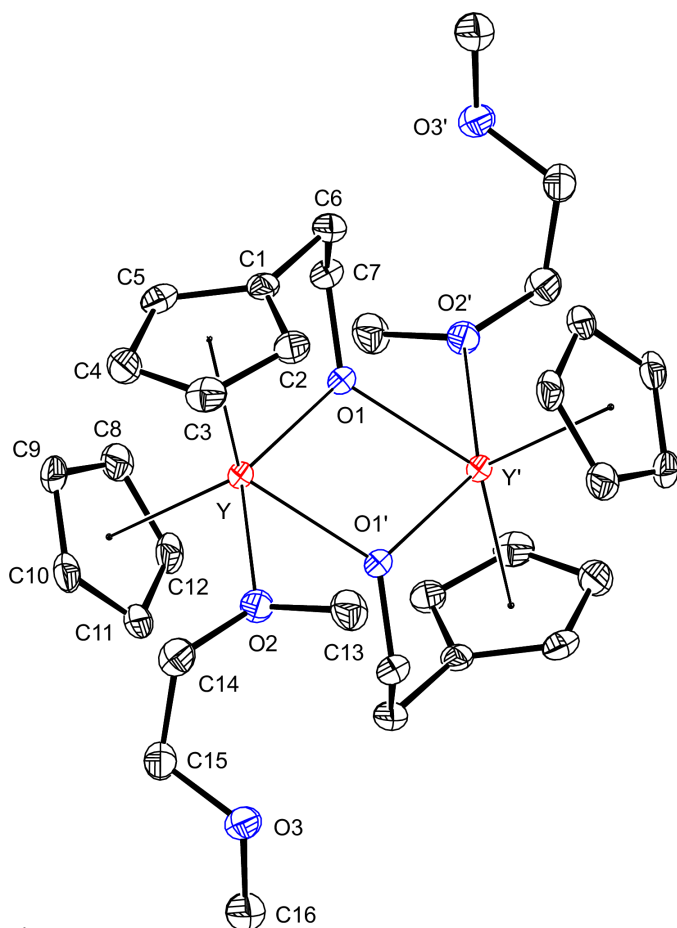
The distances of the Y atom to the cyclopentadienyl-ring centroids are in good agreement with the distances found in  $\text{Cp}_3\text{Y}(\text{THF})$  (2.438, 2.453 and 2.454 Å; Rogers *et al.*, 1981).

The O–Y–O<sup>i</sup> [symmetry code: (i)  $1-x, 1-y, 1-z$ ] bond angle of the central Y<sub>2</sub>O<sub>2</sub> ring is somewhat smaller than

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**Figure 1**  
The molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level.

in the above described alkoxide complexes  $[(\text{Me}_3\text{SiC}_5\text{H}_4)_2\text{Y}(\mu\text{-OMe})_2]$  [73.6 (1) $^\circ$ ; Evans *et al.*, 1992],  $[(\text{MeC}_5\text{H}_4)_2\text{Y}(\mu\text{-O}^i\text{Pr})_2]$  [74.86(7) $^\circ$ ; Li *et al.*, 2000] and  $[(\text{MeC}_5\text{H}_4)_2\text{Y}(\mu\text{-OCH=CH}_2)_2]$  [73.1(1) $^\circ$ ; Evans *et al.*, 1986]. The  $\text{Y}_2\text{O}_2$  ring is perfectly planar.

Due to the trigonal bipyramidal coordination geometry of the metal atom, the angle formed by the central yttrium atom and the two ring centroids is smaller than in the related tetrahedral complex  $[(\text{MeC}_5\text{H}_4)_2\text{Y}(\mu\text{-O}^i\text{Pr})_2]$  (124.0 $^\circ$ ; Li *et al.*, 2000).

## Experimental

A solution of 2,4-cyclopentadiene-1-ethanol (0.22 g, 2.0 mmol; Ohta *et al.*, 1977) in THF (5 ml) was added to  $\text{Cp}_3\text{Y}$  (0.57 g, 2.0 mmol) in THF (10 ml), and the mixture was stirred for 15 min at ambient temperature until  $\text{Cp}_3\text{Y}$  was completely dissolved. The solution was concentrated to 3 ml and hexane (10 ml) was added. After centrifuging the mixture, the resultant white microcrystalline solid of the title compound was separated by decantation, washed with hexane (10 ml) and dried in vacuum (yield 0.51 g, 72%). Suitable crystals were obtained by recrystallization from dme (m.p. 385–388 K). Spectroscopic analysis, IR (Nujol,  $\nu$   $\text{cm}^{-1}$ ): 3060 (w), 1360 (m), 1040 (s), 890 (m), 780 (s), 730 (m), 520 (w); elemental analysis, calculated for  $\text{C}_{32}\text{H}_{46}\text{O}_6\text{Y}_2$ : Y 25.26%; found: 25.08%.

## Crystal data

$[\text{Y}_2(\text{C}_5\text{H}_5)_2(\text{C}_7\text{H}_8\text{O})_2(\text{C}_4\text{H}_{10}\text{O}_2)_2]$   
 $M_r = 704.51$   
 Monoclinic,  $P2_1/n$   
 $a = 8.6073$  (2)  $\text{\AA}$   
 $b = 11.2146$  (1)  $\text{\AA}$   
 $c = 15.7840$  (1)  $\text{\AA}$   
 $\beta = 92.751$  (1) $^\circ$   
 $V = 1521.83$  (4)  $\text{\AA}^3$   
 $Z = 2$

$D_x = 1.537$   $\text{Mg m}^{-3}$   
 Mo  $K\alpha$  radiation  
 Cell parameters from 5194 reflections  
 $\theta = 2.2\text{--}30.6^\circ$   
 $\mu = 3.84$   $\text{mm}^{-1}$   
 $T = 173$  (2) K  
 Block, colorless  
 $0.40 \times 0.38 \times 0.30$  mm

## Data collection

Siemens SMART CCD diffractometer  
 $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.448$ ,  $T_{\max} = 0.659$   
 11 359 measured reflections

3482 independent reflections  
 2489 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.081$   
 $\theta_{\text{max}} = 27.5^\circ$   
 $h = -10 \rightarrow 11$   
 $k = -13 \rightarrow 14$   
 $l = -15 \rightarrow 20$

## Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.045$   
 $wR(F^2) = 0.088$   
 $S = 1.01$   
 3482 reflections  
 183 parameters

H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0324P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.59$   $\text{e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.47$   $\text{e \AA}^{-3}$

**Table 1**

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

Cg1 and Cg2 are the centroids of the C1–C5 and C8–C12 rings, respectively.

Y–Cg1	2.4537 (19)	Y–C4	2.761 (4)
Y–Cg2	2.4260 (17)	Y–C5	2.690 (3)
Y–O1 <sup>i</sup>	2.265 (2)	Y–C8	2.690 (4)
Y–O1	2.280 (2)	Y–C9	2.704 (3)
Y–O2	2.481 (2)	Y–C10	2.714 (3)
Y–C1	2.687 (3)	Y–C11	2.714 (3)
Y–C2	2.722 (4)	Y–C12	2.700 (4)
Y–C3	2.792 (4)		
Cg1–Y–Cg2	120.80 (6)	Cg2–Y–O1 <sup>i</sup>	105.33 (7)
Cg1–Y–O1	94.49 (7)	Cg2–Y–O2	104.72 (7)
Cg1–Y–O1 <sup>i</sup>	133.80 (7)	O1 <sup>i</sup> –Y–O1	69.17 (9)
Cg1–Y–O2	93.85 (7)	O1 <sup>i</sup> –Y–O2	75.83 (8)
Cg2–Y–O1	105.56 (7)	O1–Y–O2	138.45 (8)

Symmetry code: (i)  $1 - x, 1 - y, 1 - z$ .

The H atoms were placed in calculated positions and assigned an isotropic displacement parameter of 0.08  $\text{\AA}^2$ . The idealized  $\text{CH}_3$  groups were allowed to rotate about their C–O bond. The geometrical aspects of the structure were analyzed using PLATON (Spek, 2001).

Data collection: SMART (Siemens, 1995); cell refinement: SAINT (Siemens, 1995); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1990); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ZORTEP (Zsolnai & Pritzkow, 1994); software used to prepare material for publication: SHELXL97.

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