

Di- $\mu$ -isopropoxy-bis[bis( $\eta^5$ -methylcyclopentadienyl)yttrium(III)]Huanrong Li,<sup>a</sup> Yingming Yao,<sup>a</sup> Qi Shen<sup>a\*</sup> and Linhong Weng<sup>b</sup><sup>a</sup>Department of Chemistry, Suzhou University, Suzhou 215006, People's Republic of China, and <sup>b</sup>Institute of Elemental-Organic Chemistry, Nankai University, Tianjing 300071, People's Republic of China

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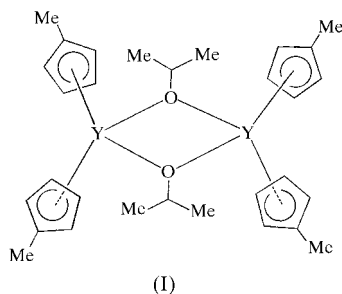
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The title complex,  $[\text{Y}_2(\text{C}_6\text{H}_7)_4(\text{C}_3\text{H}_7\text{O})_2]$ , is a centrosymmetric dimer bridged through the O atoms of the isopropoxide ligands. The  $\text{Y}_2\text{O}_2$  unit is planar and the geometry around the eight-coordinate Y atom is distorted pseudo-tetrahedral. The Y—O distances are 2.2228 (19) and 2.2432 (19) Å, and the O—Y—O angle is 74.86 (7)°.

## Comment

Lanthanide alkoxides have been used in a variety of applications, including as homogeneous catalysts for organic synthesis and polymerization (Shibasaki *et al.*, 1997; Shen *et al.*, 1995) and in the preparation of high purity oxide materials (Hubert-Pfalzgraf, 1995). In our study of the catalytic properties of organolanthanide alkoxides, the title complex, (I), was obtained from the reaction of  $\text{Cp}'_3\text{Y}$  ( $\text{Cp}' = \text{CH}_3\text{C}_5\text{H}_4$ ) with an equimolar amount of isopropyl alcohol in tetrahydrofuran.



In the crystal, (I) is found to be a centrosymmetric binuclear molecule, with the isopropoxide ligands as the bridging groups. This is similar to other binuclear bis(cyclopentadienyl)lanthanide alkoxides (Wu *et al.*, 1992, 1994; Evans *et al.*, 1986). The eight-coordinate metal centres are coordinated to two methylcyclopentadienyl ring centroids and two isopropoxide O atoms to form a distorted tetrahedral geometry.

The Y1—O1 distance in (I) [2.2228 (19) Å] is much longer than that observed for the Yb—O bond in  $[(\text{C}_5\text{H}_5)_2\text{Yb}(\mu\text{-OCH}_2\text{CH}_2\text{CH}_3)_2]$  [2.1970 (5) Å; Wu *et al.*, 1992] and a little shorter than the Y—O bond in  $[(\text{MeC}_5\text{H}_4)_2\text{Y}(\mu\text{-OCH}=\text{CH}_2)]$

[2.275 (3) Å; Evans *et al.*, 1986], but is similar to the value accepted for the Y—O bond in  $[(\text{C}_5\text{H}_4\text{SiMe}_3)_2\text{Y}(\mu\text{-OMe})_2]$  [2.2170 (3) Å; Evans *et al.*, 1992]. The bond angle O1—Y1—O1( $-x, 2-y, 1-z$ ) in (I) [74.86 (7)°] is slightly larger than that found in related complexes, such as  $[(\text{C}_5\text{H}_5)_2\text{Yb}(\mu\text{-OCH}_2\text{CH}_2\text{CH}_3)_2]$  [73.6 (2)°; Wu *et al.*, 1992],  $[(\text{MeC}_5\text{H}_4)_2\text{Y}(\mu\text{-OCH}=\text{CH}_2)_2]$  [73.1 (7)°; Evans *et al.*, 1986] and  $[(\text{C}_5\text{H}_4\text{-SiMe}_3)_2\text{Y}(\mu\text{-OMe})_2]$  [73.6 (1)°; Evans *et al.*, 1992]. However, the bond angle Y—O—Y( $-x, 2-y, 1-z$ ) [105.14 (7)°] is much smaller than those found in the corresponding related  $(\text{Cp}'_2\text{LnOR})_2$  structures (Ln = Y, Yb, Ce), such as  $[(\text{MeC}_5\text{H}_4)_2\text{Y}(\mu\text{-OCH}=\text{CH}_2)_2]$  [106.9 (1)°; Evans *et al.*, 1986] and  $[(\text{C}_5\text{H}_4\text{SiMe}_3)_2\text{Y}(\mu\text{-OMe})_2]$  [106.4 (1)°; Evans *et al.*, 1992].

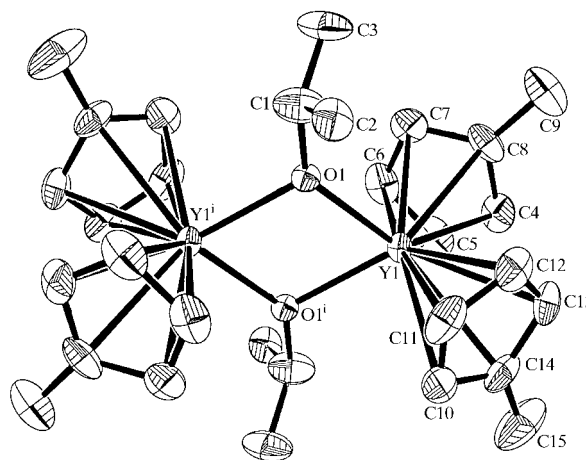


Figure 1

The molecular structure of (I) showing 40% probability displacement ellipsoids. H atoms have been omitted for clarity; symmetry code as in Table 1.

## Experimental

The organolanthanide complex described in this paper is very sensitive to air and moisture. Consequently, all manipulations were carried out under argon by Schlenk techniques. Crystals of (I) were obtained by the reaction of  $\text{YCp}'_3$  with one equivalent of isopropyl alcohol in tetrahydrofuran, followed by crystallization from a toluene solution at 263 K. A suitable crystal was sealed in a thin-walled glass capillary for single-crystal structure determination.

## Crystal data

$[\text{Y}_2(\text{C}_6\text{H}_7)_4(\text{C}_3\text{H}_7\text{O})_2]$   
 $M_r = 612.46$   
 Monoclinic,  $P2_1/n$   
 $a = 9.8370$  (8) Å  
 $b = 12.3820$  (9) Å  
 $c = 12.1515$  (9) Å  
 $\beta = 97.212$  (2)°  
 $V = 1468.36$  (19) Å<sup>3</sup>  
 $Z = 2$

$D_x = 1.385$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 Cell parameters from 4567 reflections  
 $\theta = 2.36\text{--}26.04^\circ$   
 $\mu = 3.955$  mm<sup>-1</sup>  
 $T = 298$  (2) K  
 Prismatic, colourless  
 $0.50 \times 0.35 \times 0.30$  mm

## Data collection

Bruker SMART CCD area-detector diffractometer  
 $\omega$  scans  
 Absorption correction: empirical (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.132$ ,  $T_{\max} = 0.305$   
 6773 measured reflections  
 3002 independent reflections

2484 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.033$   
 $\theta_{\text{max}} = 26.40^\circ$   
 $h = -12 \rightarrow 12$   
 $k = -9 \rightarrow 15$   
 $l = -14 \rightarrow 15$   
 Intensity decay: 9.6%

## Refinement

Refinement on $F^2$	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.036$	$w = 1/[\sigma^2(F_o^2) + (0.0628P)^2]$
$wR(F^2) = 0.099$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.086$	$(\Delta/\sigma)_{\max} = 0.002$
3002 reflections	$\Delta\rho_{\max} = 0.89 \text{ e } \text{\AA}^{-3}$
154 parameters	$\Delta\rho_{\min} = -0.82 \text{ e } \text{\AA}^{-3}$

**Table 1**  
Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

Y1—O1	2.2228 (19)	Y1—C5	2.661 (4)
Y1—O1 <sup>i</sup>	2.2432 (19)	Y1—C7	2.667 (3)
Y1—C11	2.641 (4)	Y1—C4	2.675 (3)
Y1—C6	2.652 (4)	Y1—C13	2.680 (3)
Y1—C12	2.653 (3)	Y1—C8	2.683 (3)
Y1—C10	2.660 (3)	Y1—C14	2.690 (4)
O1—Y1—O1 <sup>i</sup>	74.86 (7)	Y1—O1—Y1 <sup>i</sup>	105.14 (7)
Cp1—Y1—Cp2	124.0		

Symmetry code: (i)  $-x, 2 - y, 1 - z$ .

H atoms were included but not refined. All calculations were performed using the *TEXSAN* (Molecular Structure Corporation, 1992) crystallographic software package.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997a); molecular graphics: *SHELXTL* (Sheldrick, 1997b); software used to prepare material for publication: *SHELXTL*.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: TA1289). Services for accessing these data are described at the back of the journal.

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