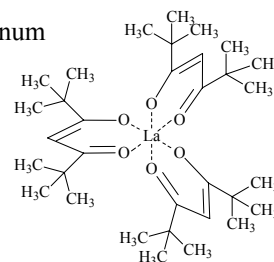


955  
ED $\text{C}_{33}\text{H}_{57}\text{LaO}_6$ **Tris(2,2,6,6-tetramethyl-3,5-heptanedionato- $\kappa\text{O},\kappa\text{O}'$ )lanthanum**  
Tris(dipivaloylmethanato- $\kappa\text{O},\kappa\text{O}'$ )lanthanumessentially  $\text{D}_3$ 

$r_g$	$\text{\AA}^a$	$\theta_\alpha$	$\text{deg}^a$
La–O	2.381(6)	O–La–O	71.4(2)
O–C	1.286(5)	C–C(r)–C	123.7(13)
C–C(r)	1.409(7)	O–C–C(t)	116.8(7)
C–C(t)	1.542(13)	C–C(t)–C(m)	109.5(5)
C(t)–C(m)	1.561(6)	C(t)–C(m)–H	109.0(4)
C(m)–H	1.115(5)	$\gamma^b$	9.1(25)
C(r)–H	1.115 <sup>c</sup>	$\tau^d$	35.6(13)
		$\phi^e$	3.0(14)
		$\varphi^f$	22.7(21)



According to the results of mass spectrometric study, the molecule exists only in the monomeric form. Local  $\text{C}_{3v}$  symmetry was assumed for methyl and *t*-butyl groups. Each methyl group was assumed to be staggered with respect to the C–C(t) bond. The nozzle temperature was 478...482(5) K.

<sup>a</sup>) 2.5 times the estimated standard errors including a systematic error.

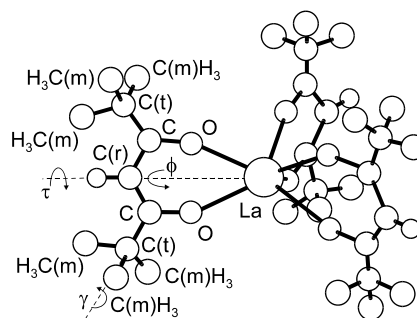
<sup>b</sup>) Torsional angle of the *t*-butyl group around the C–C(t) bond,  $\gamma = 0^\circ$  when one C(t)–C(m) bond is eclipsed with respect to the C–C(r) bond.

<sup>c</sup>) Assumed.

<sup>d</sup>) Torsional angle of the ligand around the  $\text{C}_2$  axis,  $\tau = 0^\circ$  when the molecule has  $\text{D}_{3h}$  symmetry.

<sup>e</sup>) Folding angle of the ligand, *i.e.*, the dihedral angle between the OLaO and OCCO planes.

<sup>f</sup>) Rotational angle of the upper triangle O...O...O atoms with respect to the lower O...O...O triangle,  $\varphi = 0^\circ$  for the  $\text{D}_{3h}$  configuration of the polyhedron.



Giricheva, N.I., Belova, N.V., Shlykov, S.A., Girichev, G.V., Vogt, N., Tverdova, N.V., Vogt, J.: J. Mol. Struct. **605** (2002) 171.