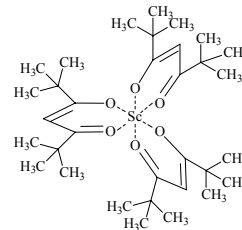


956  
ED $C_{33}H_{57}O_6Sc$ 

**Tris(2,2,6,6-tetramethyl-3,5-heptanedionato- $\kappa O, \kappa O'$ )scandium(III)**  
 Tris(dipivaloylmethanato- $\kappa O, \kappa O'$ )scandium(III)

 $D_3$ 

$r_g$	$\text{\AA}^a$	$\theta_\alpha$	$\text{deg}^a$
Sc–O	2.074(5)	O–Sc–O	82.4(4)
O–C	1.278(3)	C–C(r)–C	123.2(15)
C–C(r)	1.395(3)	O–C–C(t)	116.1(6)
C–C(t)	1.537(3)	C–C(t)–C(m)	108.7(4)
C(t)–C(m)	1.547(4)	Sc–O–C	132.3(13)
C(m)–H	1.111(3)	C(t)–C(m)–H	110.2(6)
C(r)–H	1.115 <sup>b</sup>	$\gamma^c$	28.8(9)
		$\tau^d$	33.4(7)
		$\phi^e$	2.3(26)
		$\varphi^f$	25.7(15)



According to the results of mass spectrometric study, the molecule exists only in the monomeric form. Local  $C_{3v}$  symmetry was assumed for the 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 134...137 °C.

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

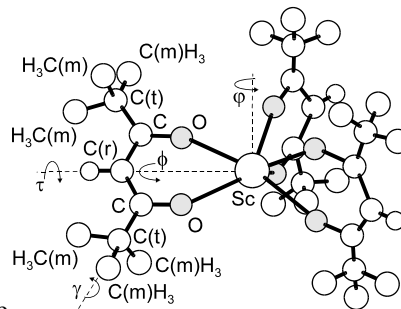
<sup>b</sup>) Assumed.

<sup>c</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>d</sup>) Torsional angle of the ligand around the  $C_2$  axis,  $\tau = 0^\circ$  when the molecule has  $D_{3h}$  symmetry.

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

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



Belova, N.V., Giricheva, N.I., Girichev, G.V., Shlykov., S.A., Tverdova, N.V., Kuz'mina, N.P., Zaitseva, I.G.: Zh. Strukt. Khim. **43** No.6 (2002) 1001; J. Struct. Chem. (Engl. Transl.) **43** (2002) 925.