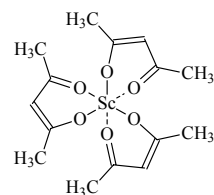


930
ED $\text{C}_{15}\text{H}_{21}\text{O}_6\text{Sc}$ **Tris(2,4-pentanedionato- $\kappa\text{O}, \kappa\text{O}'$)scandium**
Scandium tris(acetylacetonate)**D₃**

r_g	Å ^{a)}
Sc–O	2.083(4)
C–O	1.277(3)
C–C(r)	1.396(4)
C–C(m)	1.513(4)
C(m)–H	1.116(11)

θ_α	deg ^{a)}
O–Sc–O	82.4(13)
Sc–O–C	132.2(15)
C–C(r)–C	123.8(15)
O–C–C(m)	116.2(15)
H–C(m)–C	107.4(13)
$\tau^b)$	35.3(10)
$\varphi^c)$	26.8(11)
$\phi^d)$	3.0(27)



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 groups. Torsion of the methyl groups around the C–C(m) bonds (torsional angle γ) was estimated to be essentially free.

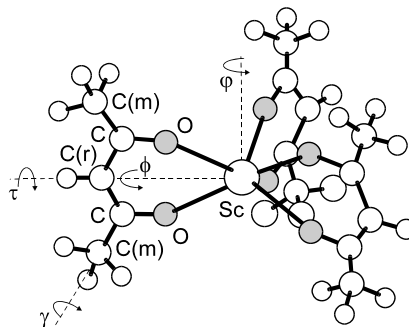
The nozzle temperature was 428(5) K.

^{a)} 2.5 times the estimated standard errors including a systematic error.

^{b)} Torsional angle of the ligand around C_2 axis, $\tau = 0^\circ$ when the molecule has D_{3h} symmetry.

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

^{d)} Folding angle of the ligand, *i.e.*, dihedral angle between the OScO and OCCO planes.



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.1 (2002) 61; J. Struct. Chem. (Engl. Transl.) **43** (2002) 56.

See also: Ezhov, Yu.S., Komarov, S.A., Sevast'yanov, V.G.: Zh. Strukt. Khim. **39** No.4 (1998) 633; J. Struct. Chem. (Engl. Transl.) **39** (1998) 514.