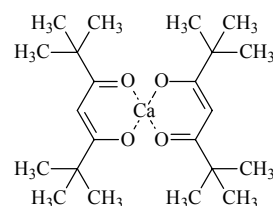


945
ED $\text{C}_{22}\text{H}_{38}\text{CaO}_4$ **Bis(2,2,6,6-tetramethyl-3,5-heptanedionato- $\kappa\text{O},\kappa\text{O}'$)calcium**
Bis(dipivaloylmethanato)calciumessentially D_{2d}

r_g	\AA^a	θ_α	deg^a
Ca–O	2.209(7)	O–Ca–O	80.6(6)
C–C(r)	1.450(7)	C(t)–C–C(r)	117.0(2)
C–C(t)	1.511(7)	C–C(r)–C	121.1(33)
C(t)–C(m)	1.575(5)	τ_1^b	92.5(51)
O–C	1.285(5)	φ^c	4.6(19)
C(m)–H	1.077 ^d	τ_2^c	0.7(23)



According to the results of a mass spectrometric study, it was assumed in the ED analysis that the only monomeric molecular form was present in the overheated vapor. Local C_{3v} symmetry was assumed for the *t*-butyl groups, and the H–C–H bond angles were assumed to be tetrahedral. The nozzle temperature was 444(2) °C.

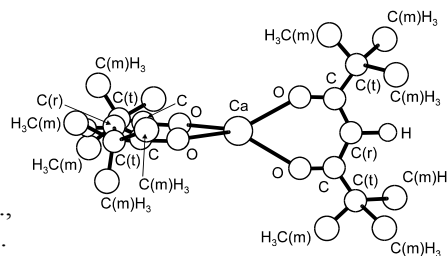
^a) 2.5 times the estimated standard errors including a systematic error.

^b) Angle of the ligand rotation about the Ca...C(r) axis; $\tau_1 = 90^\circ$ when the ligand planes are perpendicular to each other (D_{2d} symmetry).

^c) Angle of ligand folding along the O...O line, *i.e.*, angle between the OCaO and OCC(r)CO planes.

^d) r_α value, uncertainty is not given in the original paper.

^e) C(m)–C(t)–C–O torsional angle; $\tau_2 = 0^\circ$ for the *syn* position.



Giricheva, N.I., Isakova, N.A., Girichev, G.V., Petrov, V.M., Kuzmina, N.P.: Zh. Strukt. Khim. **40** No.3 (1999) 468; J. Struct. Chem. (Engl. Transl.) **40** (1999) 387.