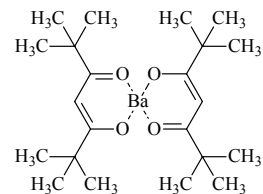


944  
ED $C_{22}H_{38}BaO_4$ **Bis(2,2,6,6-tetramethyl-3,5-heptanedionato- $\kappa O, \kappa O'$ )barium**  
Bis(dipivaloylmethanato- $\kappa O, \kappa O'$ )barium $D_{2d}$  (without methyl groups)

$r_g$	$\text{\AA}^a$
Ba–O	2.543(7)
C–C(r)	1.435(8)
C–C(t)	1.536(4)
C(t)–C(m)	1.562(10)
C(m)–H	1.130(5)
C(r)–H	1.115 <sup>b</sup>
O–C	1.290(6)

$\theta_\alpha$	deg <sup>a</sup>
O–Ba–O	66.1(5)
O–C–C(t)	117.5(8)
C–C(r)–C	121.4(13)
C(r)–C–C(t)	116.9(2)
C–C(t)–C(m)	111.9(10)
C(t)–C(m)–H	109.5 <sup>b</sup>
$\tau_1$ <sup>c</sup>	0.0(30)
$\varphi$ <sup>d</sup>	0.0(50)
$\tau_2$ <sup>c</sup>	38.4(33)



According to the results of mass spectrometric study, the vapor contained less than 1% of dimeric molecules. Therefore it was assumed in the ED analysis that only the monomer was present in the overheated vapor. Local  $C_{3v}$  symmetry was assumed for the methyl and *t*-butyl groups.

The nozzle temperature was 488(5) °C.

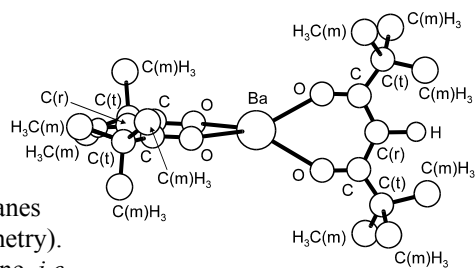
<sup>a</sup>) 2.5 times the estimated standard errors including a systematic error.

<sup>b</sup>) Assumed.

<sup>c</sup>) Angle of the ligand rotation about the Ba...C(r) axis;  $\tau_1 = 0^\circ$  when the ligand planes are perpendicular to each other ( $D_{2d}$  symmetry).

<sup>d</sup>) Angle of ligand folding along the O...O line, *i.e.*, angle between the OBaO and OCC(r)CO planes.

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



Giricheva, N.I., Girichev, G.V., Belova, N.V., Isakova, N.A., Kuzmina, N.P., Kaul, A.R., Petrov, V.M.: Zh. Strukt. Khim. **40** No.4 (1999) 647; J. Struct. Chem. (Engl. Transl.) **40** (1999) 527.