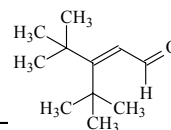


899  $C_{11}H_{20}O$ ED, *ab initio*  
calculations

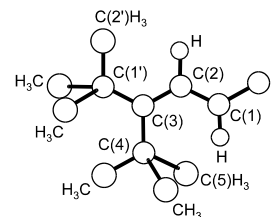
3-(1,1-Dimethylethyl)-4,4-dimethyl-2-pentalenal

essentially  $C_s$ 

$r_a$	$\text{\AA}^a$	$\theta^b$	$\text{deg}^a$
C(1)=O	1.221(2)	C(1)–C(2)=C(3)	132.6(7)
C(2)=C(3)	1.323(4)	C(2)–C(1)=O	116.7(9)
C(1)–C(2)	1.518(10)	C(2)=C(3)–C(1')	117.9(2)
C(3)–C(1') <sup>c)</sup>	1.569(4)	C(3)–C(1')–C(2') <sup>c)</sup>	111.7(3)
C–C(methyl) <sup>d)</sup>	1.530(2)	C(2)=C(3)–C(1')–C(2') <sup>c)</sup>	–4.8(7)
C(methyl)–H <sup>d)</sup>	1.096(2)	C(2)=C(3)–C(4)–C(5) <sup>c)</sup>	53.4(9)

The molecule was found to exist as a single conformer with the O=C–C=C unit in the *anti* position and two *t*-butyl groups in the nearly staggered and eclipsed positions with respect to the C(3)=C(2) bond. All C–C–H bond angles were assumed at the values from HF/6-31G\* calculations.

The nozzle temperature was 66 °C.



<sup>a)</sup> Uncertainties were unidentified, probably estimated standard errors.

<sup>b)</sup> Unidentified, possibly  $\theta_a$ .

<sup>c)</sup> Differences between the C(3)–C(1') and C(3)–C(4) bond lengths, in the C(3)–C–C(methyl) and C(2)=C(3)–C bond angles, in the C(2)=C(3)–C(1')–C and C(2)=C(3)–C(4)–C torsional angles were assumed at the values from HF/6-31G\* calculations.

<sup>d)</sup> Assumed to be all equal.

Hopf, H., Mlynek, C., Klein, D., Traetteberg, M., Bakken, P.: Eur. J. Org. Chem. (2001)1385.