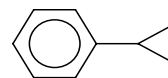
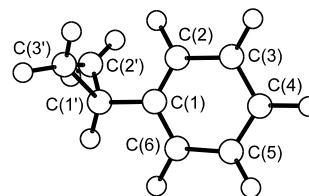


**870**      **C<sub>9</sub>H<sub>10</sub>****Cyclopropylbenzene****C<sub>s</sub>** (see comment)ED, MW, *ab initio* and DFT calculations

$r_g$	Å <sup>a)</sup>	$\theta_\alpha$	deg <sup>a)</sup>
C–H (average)	1.093(6)	C(1)–C(1')–C(2')	119.6(17)
C(2')–C(3')	1.507(26)	C(2)–C(1)–C(1')	122.5(25)
C(1')–C(2')	1.514(20)	C(1)–C(2)–C(3)	120.9(35)
C(1)–C(1')	1.520(25)	H–C(2')–C(3')	116.7(20)
C–C (ring)	1.395(1)	H–C–C (ring)	120 <sup>b)</sup>

From the following observations by pulsed-jet MW experiments, the molecule was found to exist in the bisected conformation, where the benzene ring plane bisects the C(2')–C(1')–C(3') angle: (1) The selection rules of the observed rotational transitions were consistent with this conformation. (2) Eight (rather than six) singly substituted <sup>13</sup>C isotopomers were observed and assigned. (3) Seven of the nine carbon atoms lie in the molecular symmetry plane. No transition from the other possible perpendicular conformer was observed.

MP2/6-311G\* and B3LYP/6-311G\* calculations showed that the bisected form was more stable (245 and 660 cal mol<sup>−1</sup>, respectively) than the perpendicular form. These two conformers could not be distinguished in the ED analysis. The nozzle temperature was 304 or 265 K.



bisected conformer

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

<sup>b)</sup> Assumed.

Shen, Q., Wells, C., Traetteberg, M., Bohn, R.K., Willis, A., Knee, J.: J. Org. Chem. **66** (2001) 5840.

Replaces [II/25D \(3, 2647\)](#)