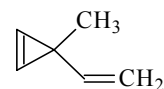


**731**      **C<sub>6</sub>H<sub>8</sub>**ED, *ab initio*  
calculations**3-Ethenyl-3-methylcyclopropene**

3-Methyl-3-vinylcyclopropene

**C<sub>s</sub> (*anti*)****C<sub>1</sub> (*gauche*)**

$r_a$	Å <sup>a)</sup>	$\theta^b$	deg <sup>a)</sup>
C(1)=C(2)	1.296(2)	M...C(3)–C(4)	122.1(3)
C(1)–C(3)	1.518(4)	C(3)–C(4)=C(5)	129.3(8)
C(3)–C(4)	1.468(4)	C(4)–C(3)–C(6)	114.8(3)
C(4)=C(5)	1.349(2)	C(1)=C(2)–H	152.3(20) <sup>c)</sup>
C(3)–C(6)	1.549(5)	C(3)–C(6)–H	110.4(23) <sup>c)</sup>
C(6)–H	1.116 <sup>d)</sup>	C(3)–C(4)–H	115.03 <sup>c)</sup>
C(5)–H	1.087(2)	C(4)=C(5)–H	125.9(33) <sup>c)</sup>



The molecule exists as a mixture of *anti* (75(3)%) and *gauche* (25%) conformers with torsional angles  $\tau[M...C(3)–C(4)=C(5)]$  of 180° and 52.2(46)°, respectively. Differences between parameters of the conformers were assumed at the values from MP2/6-31G\* calculations, and staggered conformation of the methyl C–H bonds with respect to the C(3)–C(4) bond was assumed. The energy difference between the *gauche* and *anti* conformers was estimated to be 1.03 kcal mol<sup>–1</sup> by the MP2/6-31G\* method. The nozzle was at room temperature.

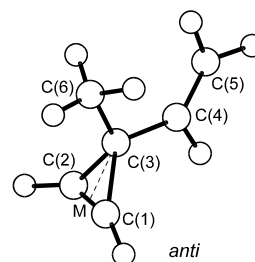
<sup>a)</sup> Estimated standard errors.

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

<sup>c)</sup> Differences between the C–C–H and C=C–H bond angles were assumed at the values from MP2/6-31G\* calculations.

<sup>d)</sup> Difference between the C–H bonds to saturated and unsaturated C atoms was assumed at the value from MP2/6-31G\* calculations.

<sup>e)</sup> Assumed at the MP2/6-31G\* value.



Bakken, P., Bolesov, I., Kuchuk, I., de Meijere, A., Mastryukov, V., Trætteberg, M.: J. Mol. Struct. **445** (1998) 107.