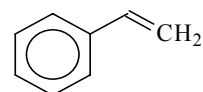


**833 C<sub>8</sub>H<sub>8</sub>**ED, *ab initio*  
calculations**Ethenylbenzene**Vinylbenzene  
Styrene**C<sub>1</sub>**

$r_a$	$\text{\AA}^a$	$\theta_a$	$\text{deg}^a$
C(1)–C(7)	1.475(23)	C(1)–C(7)=C(8)	126.9(24)
C(7)=C(8)	1.355(16)	C(2)–C(1)–C(7)	122.0 <sup>b)</sup>
C–C (ring) <sup>c)</sup>	1.399(3)	C(2)–C(1)–C(6)	118.5 <sup>d)</sup>
C(1)–C(2)	1.405(3) <sup>e)</sup>	C(1)–C(2)–C(3)	120.6 <sup>d)</sup>
C(2)–C(3)	1.395(3) <sup>e)</sup>	C(2)–C(3)–C(4)	120.3 <sup>d)</sup>
C(3)–C(4)	1.398(3) <sup>e)</sup>	C(3)–C(4)–C(5)	119.6 <sup>d)</sup>
C–H <sup>c)</sup>	1.100(7)	C(4)–C(5)–C(6)	120.1 <sup>d)</sup>
		C(1)–C(6)–C(5)	120.9 <sup>d)</sup>
		$\tau^f)$	28(21)

The experimental data were consistent with the results of MP2/6-31G\* calculations which described the vinyl torsional motion in terms of a double-minimum potential function with barriers of 0.24 and 2.73 kcal mol<sup>−1</sup> at the planar ( $\tau = 0^\circ$ ) and the perpendicular ( $\tau = 180^\circ$ ) positions, respectively, and with the minimum energy at  $\tau = 27^\circ$ . The nozzle temperature was 303...305 °C.

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

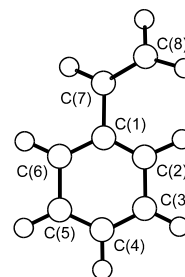
<sup>b)</sup> Assumed.

<sup>c)</sup> Average value.

<sup>d)</sup> The C–C–C (ring) and C–C–H (ring) angles were assumed at the *ab initio* values.

<sup>e)</sup> Differences in the C–C bond lengths of the ring were assumed at the value from MP2/6-31G\* calculations.

<sup>f)</sup> Torsional angle C(2)–C(1)–C(7)=C(8) from the *syn* position.



Cochran, J.C., Hagen, K., Paulen, G., Shen, Q., Tom, S., Trætteberg, M., Wells, C.: J. Mol. Struct. **413-414** (1997) 313.

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