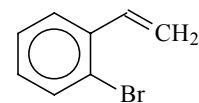


827 **C₈H₇Br**ED, *ab initio*
calculations**1-Bromo-2-ethenylbenzene**

2-Bromostyrene

C₁

r_g	\AA^a	θ_α	deg^a
C–H (average)	1.109(13)	Br–C(2)–C(3)	117.3(5)
C(1')=C(2')	1.328(21)	C(1)–C(1')=C(2')	130.4(37)
C(1)–C(1')	1.478(11)	C(1')–C(1)–C(2)	121.8(11)
C–C (ring) ^{c)}	1.405(3)	C–C–H (average)	120 ^{b)}
C–Br	1.913(6)	τ^d	152(20)

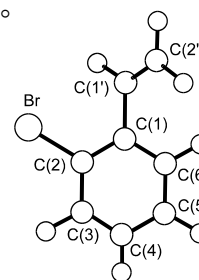
The molecule was found to exist as a nonplanar conformer with $\tau \approx 150^\circ$, but the presence of a small amount of the second conformer with $\tau \approx 54^\circ$ could not be excluded. According to the results of MP2/6-311G(d) calculations, the latter conformer is less stable by 2.52 kcal mol⁻¹. The nozzle temperature was 376...378 K.

^{a)} Twice the estimated standard errors including a systematic error.

^{b)} Constrained to the value from MP2/6-311G(d) calculations.

^{c)} Average value.

^{d)} Torsional angle C(2')=C(1')–C(1)–C(2).



Shen, Q., Kuhns, J., Hagen, K., Richardson, A.D.: J. Mol. Struct. **567-568** (2001) 73.