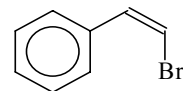


829 **C₈H₇Br**ED, *ab initio*
calculations**(Z)-(2-Bromoethenyl)benzene***cis-β*-Bromostyrene**C₁**

r_a	Å ^{a)}	θ_a	deg ^{a)}
C(1)–C(7)	1.465(20)	C(1)–C(7)=C(8)	132.8(23)
C(7)=C(8)	1.331(20)	C(2)–C(1)–C(7)	123.9(33)
C–C (ring) ^{b)}	1.400(2)	C=C–Br	125.7(15)
C–H ^{b)}	1.082(13)	C–C–C (ring)	120 ^{c)}
C–Br	1.893(8)	C–C–H (ring)	120 ^{c)}
		C(1)–C(7)–H	114.7 ^{c)}
		C(7)=C(8)–H	121.4 ^{c)}
		τ^d	29(14)

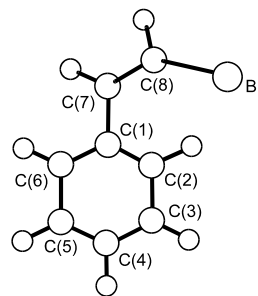
The experimental data were consistent with the results of HF/6-31G* calculations which described the vinyl torsional motion in terms of a double-minimum potential function with barriers of 0.43 and 1.10 kcal mol^{−1} at the planar ($\tau = 0^\circ$) and the perpendicular ($\tau = 180^\circ$) positions, respectively, and with the minimum energy at $\tau = 39^\circ$. The nozzle temperature was 338...340 °C.

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

^{b)} Average value.

^{c)} Assumed at the *ab initio* value.

^{d)} 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.