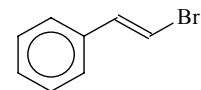
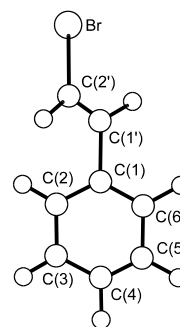


**828**      **C<sub>8</sub>H<sub>7</sub>Br**ED, *ab initio*  
calculations**(*E*)-(2-Bromoethenyl)benzene***trans*- $\beta$ -Bromostyrene**C<sub>1</sub>**

$r_g$	Å <sup>a)</sup>	$\theta_\alpha$	deg <sup>a)</sup>
C–H (average)	1.080(13)	Br–C(2')=C(1')	122.5(16)
C(1')=C(2')	1.344(23)	C(1)–C(1')=C(2')	124.6(21)
C(1)–C(1')	1.475(12)	C(1')–C(1)–C(2)	122.0 <sup>b)</sup>
C–C (ring) <sup>c)</sup>	1.396(2)	C–C–H (average)	120 <sup>b)</sup>
C–Br	1.884(9)	$\tau$ <sup>d)</sup>	40(10)

The molecule was found to exist as a nonplanar conformer.

The nozzle temperature was 373...393 K.

<sup>a)</sup> Twice the estimated standard errors including a systematic error.<sup>b)</sup> Constrained to the value from MP2/6-311G(d) calculations.<sup>c)</sup> Average value.<sup>d)</sup> 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.