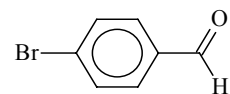


**775 C<sub>7</sub>H<sub>5</sub>BrO**

 ED, *ab initio*  
calculations

**4-Bromobenzaldehyde**
*p*-Bromobenzaldehyde

**C<sub>s</sub>**


$r_g$	Å <sup>a)</sup>	$\theta_a$	deg <sup>a)</sup>
C(1)–C(2)	1.401(2)	C(3)–C(4)–C(5)	121.2(2)
C(4)–Br	1.891(3)	C(2)–C(1)–C(7)	119.2(20)
C(1)–C(7)	1.499(13)	C(1)–C(7)=O	125.3(20)
C(7)=O	1.216(10)	C(1)–C(7)–H	114.9 <sup>b)</sup>
C–H (mean)	1.102(10)	C(6)–C(1)–C(2)	121.5(9) <sup>c)</sup>
C(2)–C(3)	1.389(2) <sup>d)</sup>	C(1)–C(2)–C(3)	120.0(2) <sup>d)</sup>
C(3)–C(4)	1.397(2) <sup>d)</sup>	C(2)–C(3)–C(4)	118.7(2) <sup>d)</sup>
C(4)–C(5)	1.391(2) <sup>d)</sup>	C(4)–C(5)–C(6)	120.6(9) <sup>c)</sup>
C(5)–C(6)	1.395(2) <sup>d)</sup>	C(5)–C(6)–C(1)	118.1(12) <sup>c)</sup>
C(1)–C(6)	1.395(2) <sup>d)</sup>		
C(7)–H	1.125(10) <sup>d)</sup>		

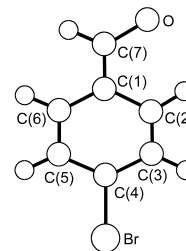
Internal rotation of the aldehyde group was described as a large-amplitude motion. The barrier to internal rotation was assumed at 37 kJ mol<sup>−1</sup> from HF/6-311G\* calculations. It was assumed that the elongation of the C–Br bond bisects the C(3)–C(4)–C(5) angle. Temperature of the measurements was 105 °C.

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

<sup>b)</sup> Assumed at the value from HF/6-311G\*\* calculations.

<sup>c)</sup> Dependent parameter.

<sup>d)</sup> Differences in the C–C(ring) and C–H bond lengths  
C–C–C angles were assumed at the values from  
HF/6-311G\*\* calculations.



Strand, T.G., Tafipol'skii, M.A., Vilkov, L.V., Volden, H.V.: Vestn. Mosk. Univ., Khim. **39** (1998) 367; Mosc. Univ. Chem. Bull. (Engl. Transl.) **53** (1998) 1.