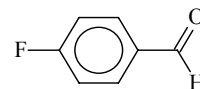


**780 C<sub>7</sub>H<sub>5</sub>FO**ED, MW, *ab initio*  
calculations**4-Fluorobenzaldehyde***p*-Fluorobenzaldehyde**C<sub>s</sub>**

$r_g$	Å <sup>a)</sup>	$\theta$ <sup>b)</sup>	deg <sup>a)</sup>
C–C (mean)	1.397(1)	C(3)–C(4)–C(5)	122.3(2)
C(1)–C(2)	1.405(1)	C(2)–C(1)–C(7)	119.0(8)
C–F	1.342(7)	C(1)–C(7)=O	125.9(10)
C(1)–C(7)	1.499(6)	C(1)–C(7)–H	114(4)
C(7)=O	1.207(5)	C(2)–C(1)–C(6) <sup>c)</sup>	121.3(7)
C–H (mean)	1.096(8)	C(1)–C(2)–C(3) <sup>c)</sup>	120.1(2)
C(2)–C(3) <sup>c)</sup>	1.393(1)	C(2)–C(3)–C(4) <sup>c)</sup>	118.1(2)
C(3)–C(4) <sup>c)</sup>	1.397(1)	C(4)–C(5)–C(6) <sup>c)</sup>	119.5(6)
C(4)–C(5) <sup>c)</sup>	1.393(1)	C(5)–C(6)–C(1) <sup>c)</sup>	118.8(9)
C(5)–C(6) <sup>c)</sup>	1.397(1)	C(3)–C(4)–F	118.7 <sup>d)</sup>
C(1)–C(6) <sup>c)</sup>	1.395(1)		
C(7)–H <sup>c)</sup>	1.121(8)		

Torsion of the formyl group was treated as a large-amplitude motion. The barrier height was assumed to be 37 kJ mol<sup>−1</sup> at the torsional angle  $\tau[C(2)–C(1)–C(7)=O] = 90^\circ$  according to the results of HF/6-311G\*\* calculations.

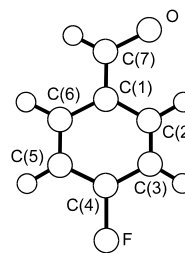
The nozzle temperature was 21 °C.

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

<sup>b)</sup> Unidentified, probably  $\theta_\alpha^0$ .

<sup>c)</sup> Dependent parameter. Difference between similar parameters was assumed at the values from MP2/6-31G\* calculations.

<sup>d)</sup> Assumed at the value from MP2/6-31G\* calculations.



Samdal, S., Strand, T.G., Tafipol'skii, M.A., Vilkov, L.V., Popik, M.V., Volden, H.V.: Vestn. Mosk. Univ., Ser. II, Khim. **38** No.5 (1997) 297.

See also: Samdal, S., Strand, T.G., Tafipolsky, M.A., Vilkov, L.V., Popik, M.V., Volden, H.V.: J. Mol. Struct. **435** (1997) 89.

ED, vibrational spectroscopy,  
*ab initio* and DFT  
calculations

**C<sub>s</sub>**, assumed

$r_e$ <sup>a)</sup>	Å <sup>b)</sup>	$\theta_e$	deg <sup>a)</sup>
C(1)–C(2)	1.397(1)	C(3)–C(4)–C(5) <sup>c)</sup>	124.7
C(2)–C(3)	1.382 <sup>c)</sup>	C(2)–C(1)–C(6)	121.6(2)
C–F	1.328(4)	C(1)–C(7)=O	125.6(7)
C(1)–C(7)	1.487(5)	C(1)–C(7)–H	113.4(40)
C(3)–C(4)	1.387 <sup>c)</sup>	C(1)–C(2)–C(3) <sup>c)</sup>	119.4
C(4)–C(5)	1.380 <sup>c)</sup>	C(2)–C(3)–C(4) <sup>c)</sup>	117.5
C(5)–C(6)	1.389 <sup>c)</sup>	C(4)–C(5)–C(6) <sup>c)</sup>	117.1
C(1)–C(6)	1.391 <sup>c)</sup>	C(5)–C(6)–C(1) <sup>c)</sup>	119.8

## Structure Data of Free Polyatomic Molecules

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C(7)=O	1.211(4)
C(2)–H	1.059(12)
C(3)–H	1.059 <sup>c)</sup>
C(5)–H	1.059 <sup>c)</sup>
C(6)–H	1.061 <sup>c)</sup>
C(7)–H	1.108(48)

ED intensities obtained previously by Samdal *et al.* were reanalyzed jointly with spectroscopic data from the literature and supported by the results of HF/6-311G\*\* calculations.

<sup>a)</sup> Anharmonic approximation with Morse-like anharmonic constants.

<sup>b)</sup> Estimated standard errors.

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

Kochikov, I.V., Tarasov, Yu.I., Spiridonov, V.P., Kuramshina, G.M., Yagola, A.G., Saakjan, A.S., Popik, M.V., Samdal, S.: J. Mol. Struct. **485-486** (1999) 421.