

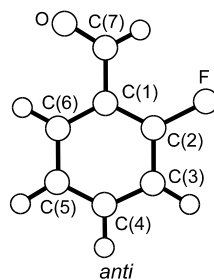
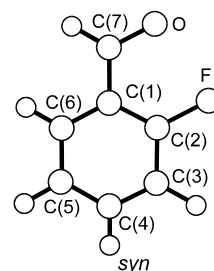
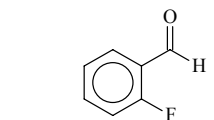
778 C₇H₅FOED, MW, *ab initio*
calculations**2-Fluorobenzaldehyde***o*-Fluorobenzaldehyde**C_s (*anti*)****C_s (*syn*)**

r_g	Å ^{a)}	θ_α	deg ^{a)}
C–C ^{b)}	1.399(2)	C(1)–C(2)–C(3)	122.0(2)
C(1)–C(2)	1.397(2)	C(2)–C(3)–C(4)	118.0(2)
C(2)–C(3)	1.393(2)	C(3)–C(4)–C(5)	120.2(2)
C(3)–C(4)	1.397(2)	C(4)–C(5)–C(6)	122.0(6)
C(4)–C(5)	1.404(2)	C(5)–C(6)–C(1)	117.5(7)
C(5)–C(6)	1.393(2)	C(6)–C(1)–C(2)	120.3(6)
C(6)–C(1)	1.408(2)	C(2)–C(1)–C(7)	121.9(6)
C(1)–C(7)	1.515(6)	C(1)–C(7)=O	122.8(6)
C–F	1.334(5)		
C(7)=O	1.216(3)		
C–H (ring)	1.090(6)		
C(7)–H	1.108(6)		

The torsion of the formyl group was treated as a large-amplitude motion. The *anti* form was found to be more stable than the *syn* form by 1.2 kcal mol^{−1}. The differences in the C–C bond lengths and in the C–C–C bond angles of the ring, between the mean value of C–H bond lengths in the ring and the C(7)–H distance were assumed at the values from HF/6-311G** calculations. The *anti* form was found to be more stable than the *syn* form by 1.2(2) kcal mol^{−1}; the corresponding *ab initio* estimate was 3.2 kcal mol^{−1}. The nozzle temperature was about 22 °C.

^{a)} 1.4 times the estimated standard errors including a systematic error.

^{b)} Mean value in the ring.



Strand, T.G., Tafipolsky, M.A., Vilkov, L.V., Volden, H.V.: J. Mol. Struct. **443** (1998) 9.

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