

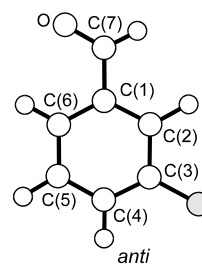
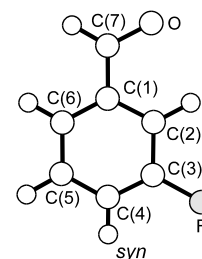
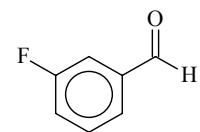
779 C₇H₅FOED, MW, *ab initio*
calculations**3-Fluorobenzaldehyde***m*-Fluorobenzaldehyde**C_s (*anti*)****C_s (*syn*)**

r_g	Å ^{a)}	θ_α	deg ^{a)}
C–C ^{b)}	1.394(2)	C(1)–C(2)–C(3)	118.3(1)
C(1)–C(2)	1.402(2)	C(2)–C(3)–C(4)	122.3(1)
C(2)–C(3)	1.382(2)	C(3)–C(4)–C(5)	119.0(1)
C(3)–C(4)	1.394(2)	C(4)–C(5)–C(6)	120.0(3)
C(4)–C(5)	1.393(2)	C(5)–C(6)–C(1)	119.9(4)
C(5)–C(6)	1.398(2)	C(6)–C(1)–C(2)	120.6(3)
C(6)–C(1)	1.396(2)	C(2)–C(1)–C(7)	118.9(9)
C(1)–C(7)	1.494(4)	C(1)–C(7)=O	126.0(4)
C–F	1.346(4)		
C(7)=O	1.201(2)		
C–H (ring)	1.103(4)		
C(7)–H	1.123(4)		

The torsion of the formyl group was treated as a large-amplitude motion. 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 energy difference between the *anti* and *syn* forms was estimated to be 0.1 kcal mol^{−1} by the HF/6-311G** method. No corresponding experimental value was reported. The nozzle temperature was *ca.* 22 °C.

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

^{b)} Mean value for the ring.



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

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