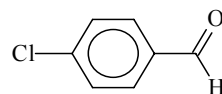


776 **C₇H₅ClO**ED, MW, *ab initio*
calculations**4-Chlorobenzaldehyde***p*-Chlorobenzaldehyde**C_s**

r_g	Å ^{a)}	θ_α	deg ^{a)}
C(1)–C(2)	1.404(1)	C(1)–C(2)–C(3)	121.8(12)
C(2)–C(3)	1.392(1) ^{b)}	C(2)–C(3)–C(4)	117.6(9)
C(3)–C(4)	1.400(1) ^{b)}	C(3)–C(4)–C(5)	121.0(5)
C(4)–C(5)	1.394(1) ^{b)}	C(2)–C(1)–C(12)	119.7(8)
C(5)–C(6)	1.398(1) ^{b)}	C(1)–C(12)=O	125.5(12)
C(6)–C(1)	1.399(1) ^{b)}	C(1)–C(12)–H	116(6)
C–Cl	1.734(3)	C(6)–C(1)–C(2)	120.2(8) ^{c)}
C(1)–C(12)	1.482(10)	C(4)–C(5)–C(6)	121.2(9) ^{c)}
C=O	1.216(5)	C(5)–C(6)–C(1)	118.2(9) ^{c)}
C–H ^{d)}	1.094(7)	C(5)–C(4)–Cl	119.5(5) ^{c)}
C(12)–H	1.117(7) ^{b)}		

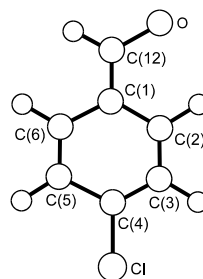
The molecule exists only as a planar conformer of C_s symmetry. The torsion of the formyl group was treated as a large-amplitude motion. The barrier height to the perpendicular orientation was assumed at the value of 37 kJ mol^{−1} from HF/6-311G* calculations. The C–Cl bond was assumed to be directed along the bisector of the C(3)–C(4)–C(5) angle. The nozzle temperature was *ca.* 64 °C.

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

^{b)} Differences in the C–C bond lengths of the ring and in the C–H bond lengths were assumed at the values from HF/6-311G* calculations.

^{c)} Dependent parameter.

^{d)} Mean value.



Møllendal, H., Gundersen, S., Tafipolsky, M.A., Volden, H.V.: J. Mol. Struct. **444** (1998) 47.