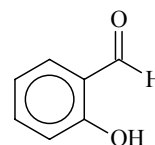


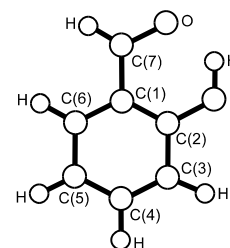
788 **C₇H₆O₂**ED, *ab initio*
calculations**2-Hydroxybenzaldehyde**

Salicylaldehyde

C_s assumed

r_g	Å ^{a)}	θ_a	deg ^{a)}
C–C (mean) ^{b)}	1.404(3)	C(1)–C(2)–C(3)	120.9(9)
C(1)–C(2) ^{c)}	1.418(14)	C(2)–C(1)–C(6)	118.2(18)
C–H (ring) ^{b)}	1.090(11)	C(1)–C(6)–C(5)	121.5(29)
C(2)–O	1.362(10)	C(4)–C(5)–C(6)	119.0(12)
O–H	0.985(14)	C(3)–C(4)–C(5)	121.5(15)
C(1)–C(7)	1.462(11)	C(2)–C(3)–C(4)	118.9(19)
C(7)=O	1.225(4)	C(1)–C(2)–O	120.9(11)
C(7)–H ^{c)}	1.11(5)	C(2)–O–H	104.8(26)
		C(2)–C(1)–C(7)	121.4(8)
		C(6)–C(1)–C(7)	120.4(8)
		C(1)–C(7)–H	116.5(37)
		O=C(7)–H	119.7(34)
		C(1)–C(7)=O	123.8(12)

The barrier height to torsion of the formyl group around the C(1)–C(7) bond was estimated to be at least 30 kJ mol^{−1} using a dynamic model within the Monte Carlo optimization scheme. All C–H bonds in the ring were assumed to be equal and directed along the bisectors of the respective C–C–C angles. The nozzle was at 68...72 °C.

^{a)} Estimated total errors.^{b)} In the benzene ring.^{c)} Differences between the C–C bond lengths in the ring, 0.019 Å maximum, and that between C(7)–H and C–H(ring) were assumed at the values from MP2(fc)/6-31G* calculations.Borisenko, K.B., Bock, C.W., Hargittai, I.: J. Phys. Chem. **100** (1996) 7426.