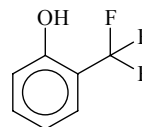


782 **C₇H₅F₃O**ED, *ab initio*
calculations**2-(Trifluoromethyl)phenol***o*-(Trifluoromethyl)phenol
o-Hydroxybenzylidene trifluoride**C_s** assumed

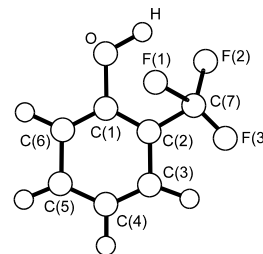
r_g	Å ^a	θ_a	deg ^a
C–C (ring) ^b	1.395(4)	O–C(1)–C(2)	121.0(12)
C–O	1.362(11)	C–O–H	105(6)
C(2)–C(7)	1.510(5)	C(7)–C(2)–C(1)	120.7(8)
C–F ^b	1.358(6)	C–C–F ^b	113.2(3)
C–H ^b	1.074(10)	τ^c	10.1(8)
O–H	0.94(2)		

Weak intramolecular bifurcated hydrogen bonding between the H atom of OH and two of the F atoms of CF₃ was indicated. Assuming the symmetric bifurcated equilibrium structure, the barrier of the CF₃ torsion was estimated from the angle τ to be 12(2) kJ mol^{–1}. The nozzle temperature was at 317...319 K.

^a) Estimated total errors.

^b) Mean value. Differences in the ring C–C and C–F bond lengths and in the C–C–F bond angles were assumed according to the results of MP2/6-31G** calculations [1].

^c) Dihedral angle F(3)–C(7)–C(2)–C(3). Effective average value over the torsional motion.



Kovács, A., Hargittai, I.: J. Phys. Chem. A **102** (1998) 3415.

[1] Kovács, A., Kolossváry, I., Csonka, G.I., Hargittai, I.: J. Comput. Chem. **17** (1996) 1804.