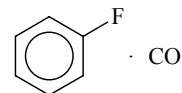


781
MW**C₇H₅FO****Fluorobenzene – carbon monoxide (1/1)**

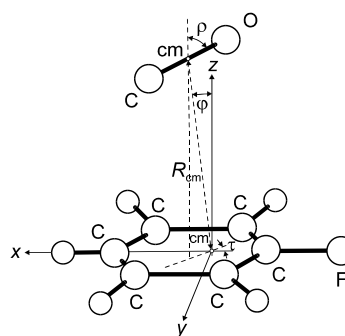
(weakly bound complex)

C_s
(effective symmetry class)
(large-amplitude motion)

r_0	Å ^{a)} ^{b)}	θ_0	deg ^{a)} ^{b)}
C≡O	1.1308 ^{c)}	φ ^{d)}	6.33(50)
R_{cm}	3.4635(50)		0.0 ^{e)}
		ρ ^{d)}	88.51(50)
		τ ^{d)} ^{f)}	61.83(50)
		θ ^{g)}	21.37(50)

r_s	Å ^{a)}	θ_s	deg ^{a)}
C≡O	1.1267(20)	φ ^{d)}	5.29(50)
R_{cm}	3.4645(50)		0.0 ^{e)}
		ρ ^{d)}	88.77(50)
		τ ^{d)} ^{f)}	60.81(50)
		θ ^{g)}	20.54(50)

Atom	a_s [Å] ^{h)}	b_s [Å] ^{h)}	c_s [Å] ^{h)}
¹³ C	2.6601	0.4113	0.5494
¹⁶ O	2.4918	0.9350	-0.4339
H ⁱ⁾	0.2635	-2.9829	^{j)}



The carbon monoxide is located above the ring plane with CO at an angle to the symmetry plane. A second set of transitions indicated that CO is executing large-amplitude motions. The rotational transitions of two states were analyzed simultaneously using an effective model Hamiltonian, which accounts for an internal rotation between CO and fluorobenzene hindered by a low barrier lower than 25 cm⁻¹.

^{a)} Uncertainties were not estimated in the original paper.

^{b)} Only differences of the moments of inertia between fluorobenzene · ¹³C¹⁶O and the remaining isotopomers were fitted.

^{c)} Constrained to the value r_0 of the free ¹³C¹⁶O.

^{d)} See figure for the definition.

^{e)} Assumed.

^{f)} Angle between the x axis and projection of the C=O bond on the ring plane.

^{g)} Angle between the symmetry axis of fluorobenzene (x axis) and the b axis of the complex.

^{h)} Coordinates in fluorobenzene·¹³C¹⁶O in the $v = 0$ state.

ⁱ⁾ Hydrogen in the 4 position of fluorobenzene.

^{j)} Imaginary.

Schäfer, M., Bauder, A.: Mol. Phys. **98** (2000) 929.