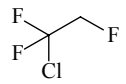
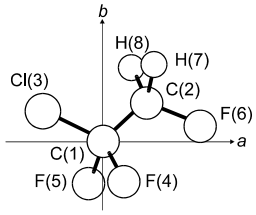
209 **$C_2H_2ClF_3$** **1-Chloro-1,1,2-trifluoroethane** **C_s**

MW, *ab initio* calculations



r_0	Å [a])	θ_0	deg [a])
C(1)–C(2)	1.516 [b])	C(1)–C(2)–F(6)	108.98 [b])
C(2)–F(6)	1.377 [b])	C(1)–C(2)–H(7,8)	109.12 [b])
C(1)–Cl(3)	1.765 [b])	C(2)–C(1)–Cl(3)	109.29 [b])
C(1)–F(4,5)	1.344(5)	C(2)–C(1)–F(4,5)	111.00(50)
C(3)–H(7,8)	1.091 [b])	F(6)–C(2)–H(7,8)	109.34 [b])
		H(7)–C(2)–H(8)	110.93 [b])
		Cl(3)–C(1)–F(4,5)	109.22(50)
		F(4)–C(1)–F(5)	107.07(5)



The conformation is staggered, and the C–Cl bond is *anti* to the C–F bond of the CH_2F group.

[a]) Uncertainties were not estimated in the original paper.
[b]) Assumed at the values from MP2/6-311+G(d,p) calculations.

Liu, B., Tatamitani, Y., Shimada, J., Ogata, T.: J. Mol. Spectrosc. **211** (2002) 99.