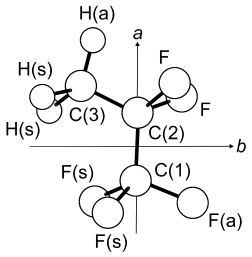
358 **$C_3H_3F_5$** **1,1,1,2,2-Pentafluoropropane** **C_s**
MW $F_3C–CF_2–CH_3$

r_0	Å [a])	θ_0	deg [a])
C(1)–C(2)	1.531(5)	C(1)–C(2)–C(3)	115.7(5)
C(2)–C(3)	1.534 [b])	C(2)–C(3)–H(a)	108.0 [b])
C(1)–F(s)	1.330 [b])	C(2)–C(3)–H(s)	109.9 [b])
C(1)–F(a)	1.338 [b])	C(2)–C(1)–F(s)	111.1 [b])
C(2)–F	1.349(5)	C(2)–C(1)–F(a)	109.9 [b])
C(3)–H(s)	1.091 [b])	C(1)–C(2)–F	106.9 [b])
C(3)–H(a)	1.090 [b])	F–C(2)–F	107.7 [b])



The barrier height to internal rotation of CF_3 was determined to be $V_3 = 2.86 \pm 0.72$ kcal mol^{-1}.

[a]) Uncertainties were not estimated in the original paper.
[b]) Assumed.

Fuchigami, K., Tatamitani, Y., Liu, B., Shimada, J., Oe, S., Ogata, T.: J. Mol. Struct. **599** (2001) 305.