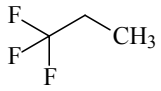
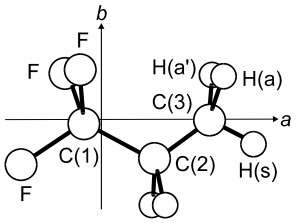
377 **$C_3H_5F_3$** **1,1,1-Trifluoropropane** **C_s**

MW



r_0	Å [a])	θ_0	deg [a])
C(1)–C(2)	1.510(5)	C(1)–C(2)–C(3)	111.23(50)
C(2)–C(3)	1.526(5)	C(2)–C(1)–F	111.87(50)
C(1)–F	1.345(5)	H–C(2)–H	106.30(100)
C(2)–H	1.094(10)	C(2)–C(3)–H(s) [b])	111.89(100)
C(3)–H(s) [b])	1.086(10)	C(2)–C(3)–H(a) [b])	110.60(100)
C(3)–H(a) [b])	1.094(10)		

The barrier to internal rotation of the methyl top was determined to be 2635(4) cal mol^{-1}.



[a]) Reasonable molecular structure derived from the rotational constants and planar moments of inertia. Uncertainties were not estimated in the original paper.

[b]) H(s) and H(a) denote the methyl hydrogen atoms in-plane and out-of-plane, respectively.

Antolínez, S., López, J.C., Alonso, J.L.: J. Chem. Soc., Faraday Trans. **93** (1997) 1291.