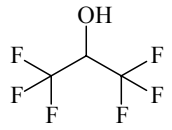
347 **$C_3H_2F_6O$** **1,1,1,3,3,3-Hexafluoro-2-propanol** **C_s**

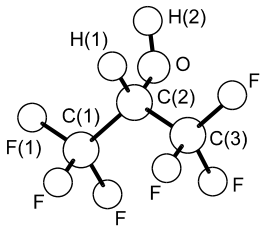
ED, vibrational spectroscopy, MM calculations



r [a])	Å [b])	θ [a])	deg [b])
C(1)–C(2)	1.527(4)	C(2)–C(1)–F(1)	104.0(3)
C(1)–F(1)	1.351(2)	C(1)–C(2)–C(3)	127.7(5)
C(2)–O	1.465(1)	C(2)–O–H(2)	135(6)
C(2)–H(1)	1.10(2)	C(1)–C(2)–H(1)	110(2)
O–H(2)	0.99(1)	τ [c])	–0.5

The molecule was found to exist as a single conformer. The barriers to torsion of the CF_3 and OH groups were estimated from results of molecular mechanics calculations to be 44.4(36) and 6.0(3) kJ mol^{-1}, respectively.
The measurements were made at room temperature.

[a]) Unidentified, probably r_a and θ_a.
[b]) Uncertainties were unidentified, possibly estimated standard errors.
[c]) Torsional angle F(1)–C(1)–C(2)–C(3), $\tau = 0°$ for the *anti* position.



Ezhov, Yu.S., Simonenko, E.P., Sevast'yanov, V.G.: Zh. Fiz. Khim. **76** No.5 (2002) 883; Russ. J. Phys. Chem. (Engl. Transl.) **76** (2002) 782.