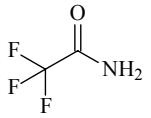
216 **$C_2H_2F_3NO$** **2,2,2-Trifluoroacetamide** **C_s** (*anti*)

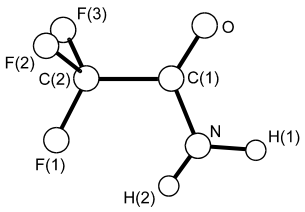
ED, *ab initio* and DFT calculations



r_g	Å [a])	θ_α	deg [a])
C=O	1.212(1)	O=C–N	126.5(2)
C–N	1.362(4)	C–C–N	116.3(4)
C–C	1.562(1)	C–N–H(1)	118.0(11)
C–F(1)	1.347(1)	C–N–H(2)	122.88 [b])
C–F(2,3)	1.333 [b])	C–C–F(1)	111.9(1)
N–H(1)	1.040(4)	C–C–F(2,3)	110.03 [b])
N–H(2)	1.037 [b])	F(1)–C–F(2)	107.58 [b])

The torsion of CF_3 group was treated as a large-amplitude motion. The *anti* conformation with τ(F(1)–C(2)–C(1)=O) torsional angle of 180° corresponds to the minimum of the potential energy curve. The barrier height to the *syn* conformation (τ = 0°) was found to be 2.7(4) kJ mol^{-1}. It agrees well with values from HF/6-311++G** and DFT/6-311++G** calculations of 2.1 and 3.0 kJ mol^{-1}, respectively.
The nozzle temperature was about 72 °C.

[a]) Estimated standard errors including a systematic error.
[b]) Differences in the similar parameters were assumed at the values from HF/6-311++G** calculations.



Gundersen, S., Samdal, S., Seip, R., Shorokhov, D.J., Strand, T.G.: J. Mol. Struct. **445** (1998) 229.