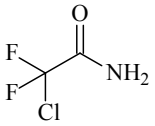
208 **$C_2H_2ClF_2NO$** **2-Chloro-2,2-difluoroacetamide** **C_1**

ED, *ab initio* and DFT calculations



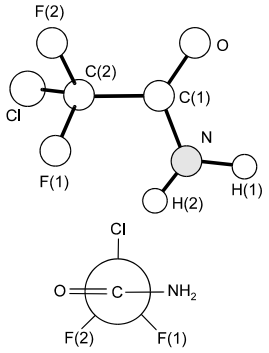
r_g	Å [a])	θ_α	deg [a])
C=O	1.214(1)	O–C–N	125.8(2)
C–N	1.366(4)	C–C–N	114.5(3)
C–C	1.568(2)	C–N–H(1)	114.1(9)
C–F(1)	1.350(2)	C–N–H(2)	118.7 [b])
C–F(2)	1.332 [b])	C–C–Cl	109.8(2)
C–Cl	1.771(2)	C–C–F(1)	110.7(1)
N–H(1)	1.048(4)	C–C–F(2)	109.5 [b])
N–H(2)	1.046 [b])	Cl–C–F(1)	109.0(1)
		Cl–C–F(2)	110.0 [b])
		τ [c])	96(6)

According to the results of HF/6-31G* and HF/6-311++G** calculations, the molecule exists as one conformer with the C–Cl bond approximately orthogonal to the CCON skeleton and a slightly nonplanar NH_2 group. The structural parameters were obtained in the ED analysis by a dynamic model considering the CF_2Cl torsion. The barrier heights were found to be 8.9(9) and 5.0(5) kJ mol^{-1} at $\tau = 0°$ and 180°, respectively. The nozzle temperature was 94 °C.

[a]) Estimated standard errors including a systematic error.

[b]) Differences between the C–F(1) and C–F(2), N–H(1) and N–H(2), C–N–H(1) and C–N–H(2), C–C–F(1) and C–C–F(2), and Cl–C–F(1) and Cl–C–F(2) parameters were assumed at the values from *ab initio* calculations.

[c]) Torsional angle Cl–C–C–N, $\tau = 0°$ for the *syn* position.



Gundersen, S., Novikov, V.P., Samdal, S., Seip, R., Shorokhov, D.J., Sipachev, V.A.: J. Mol. Struct. **485-486** (1999) 97.