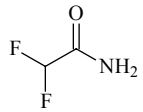
243 $C_2H_3F_2NO$ 2,2-Difluoroacetamide C_1

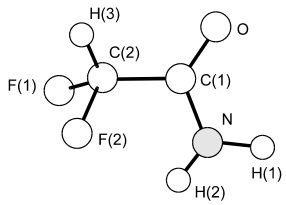
ED, *ab initio* and DFT calculations

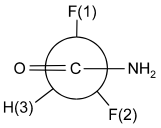


r_g	Å [a])	θ_a	deg [a])
C=O	1.212(1)	O=C–N	126.5(5)
C–N	1.352(7)	C–C–N	114.3(3)
C–C	1.535(2)	C–N–H(1)	122.0(10)
C–H(3)	1.113(8)	C–N–H(2)	125.4 [b])
C–F(1)	1.358(3)	C–C–H(3)	111.6
C–F(2)	1.365 [b])	C–C–F(1)	109.9(2)
N–H(1)	1.051(4)	C–C–F(2)	112.2 [b])
N–H(2)	1.049 [b])	H(3)–C–F(1)	107.9(3)
		H(3)–C–F(2)	107.9 [b])
		τ [c])	35(1)

According to results of HF/6-311++G**, MP2/6-311++G** and B3LYP/6-311++G** calculations, the molecule exists as one conformer with one of the C–F bonds approximately orthogonal to the CCON skeleton plane. The barrier height was found from ED data to be 2.8(5) kJ mol^{-1} at $\tau = 0°$.

The nozzle temperature was about 100 °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 H(3)–C–F(1) and H(3)–C–F(2) parameters were assumed at the values from HF/6-311++G** calculations.

[c]) Torsional angle O=C–C–H(3), $\tau = 0°$ for the *syn* position.

Gundersen, S., Samdal, S., Seip, R., Shorokhov, D.J.: J. Mol. Struct. **477** (1999) 225.