

334 **C₃F₂N₂O₂**
ED, *ab initio* and DFT
calculations

DifluorodiisocyanatomethaneC₁ (conformer I)C₂ (conformer II)

r_a	Å ^{a)}	θ_a	deg ^{a)}
C–F	1.354(2)	N–C(1)–N	111.6(13)
C–N	1.407(3)	F–C(1)–F	106.4 ^{b)}
N=C(2,2')	1.207(2)	C(1)–N=C(2') ^{c)}	127.7(12)
C=O	1.168(3)	C(1)–N=C(2) ^{c)}	127.1(12)
		N=C(2,2')=O ^{d)}	171.7(26)
		τ_1 ^{e)}	131(4)
		τ_2 ^{f)}	43(5)

The molecule was found to exist as a mixture of two conformers with C₁ symmetry (72(2)%) and C₂ symmetry (28(2)%). Differences between the corresponding bond lengths and angles of these conformers were constrained to the values from MP2/6-311G(2df) calculations. The parameters are listed for the conformer with C₁ symmetry (conformer I). Effective torsional angles were determined for both conformers ($\tau(\text{N–C(1)–N=C(2,2')}) = 52(8)^\circ$ for the conformer with C₂ symmetry); these angles may deviate from equilibrium values by up to *ca.* 20°. The C(1)–N=C(2,2')=O moieties were assumed to be planar. The nozzle was at room temperature.

^{a)} Three times the estimated standard errors.

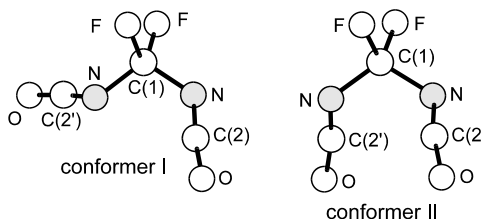
^{b)} Assumed at the value from MP2/6-311G(2df) calculations.

^{c)} Difference between the C(1)–N=C angles was assumed at the value from MP2/6-311G(2df) calculations.

^{d)} The N=C=O angles were assumed to be equal. The bent occurs in the C(1)–N=C(2, 2')=O plane away from the opposite C(1)–N bond.

^{e)} Torsional angle N–C(1)–N=C(2') from the *syn* position.

^{f)} Torsional angle N–C(1)–N=C(2) from the *syn* position.



Buschmann, J., Lentz, D., Luger, P., Röttger, M., Oberhammer, H.: J. Phys. Chem. A **104** (2000) 7123.