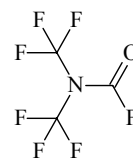
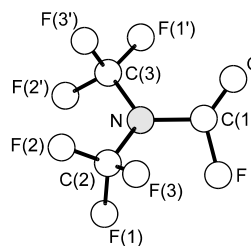


338 C₃F₇NOED, *ab initio* and DFT calculations**Bis(trifluoromethyl)carbamoyl fluoride****C₁**

r_a	Å ^{a)}	θ_a	deg ^{a)}
C–F (mean)	1.328(2)	N–C(1)=O	129.4(15)
$\Delta(\text{C–F})$ ^{b)}	0.008 ^{c)}	N–C(1)–F	105.7(24)
C(2,3)–F	1.327(3)	F–C–F	108.5(2)
C(1)–F	1.335(5)	C(1)–N–C(2)	121.4(7) ^{d)}
N–C(1)	1.394(15)	C(1)–N–C(3)	122.6(7) ^{d)}
N–C(2,3)	1.451(4)	C(2)–N–C(3)	115.5(11)
C=O	1.182(6)	$\Sigma\alpha(\text{N})$ ^{e)}	359.5(3)
		tilt(CF ₃) ^{f)}	1.2(12)
		τ_1 ^{g)}	37.2(27)
		τ_2 ^{h)}	28.6(36)
		τ_3 ⁱ⁾	32.9(39)
		τ_4 ^{j)}	97.9(27)
		τ_5 ^{k)}	–166.5(32)



The nozzle was at room temperature.

^{a)} Three times the estimated standard errors.^{b)} [C(1)–F] – [C(2,3)–F].^{c)} Constrained to the value from MP2/6-311G* calculations.^{d)} Difference between C(1)–N–C bond angles was assumed at the value from MP2/6-311G* calculations.^{e)} Sum of the angles around nitrogen.^{f)} Tilt angle between the C₃ axis of CF₃ group in the C(2)NC(3) plane away from the opposite CF₃ group.^{g)} Torsional angle F–C(1)–N–C(2), $\tau_1 = 0^\circ$ for the *syn* position.^{h)} Torsional angle O=C(1)–N–C(3), $\tau_2 = 0^\circ$ for the *syn* position.ⁱ⁾ Torsional angle lp–N–C=O, where lp is lone pair; zero position when the nitrogen lone pair is perpendicular to the COF plane.^{j)} Torsional angle C(3)–N–C(2)–F(1), $\tau_4 = 0^\circ$ for the *syn* position.^{k)} Torsional angle C(2)–N–C(3)–F(1'), $\tau_5 = 0^\circ$ for the *syn* position.Trautner, F., Reinemann, S., Minkwitz, R., Oberhammer, H.: J. Am. Chem. Soc. **122** (2000) 4193.