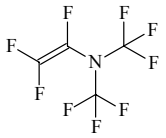
479 **C_4F_9N** **1,2,2-Trifluoro-*N*,*N*-bis(trifluoromethyl)-ethenamine** essentially C_s

ED, *ab initio* and DFT calculations

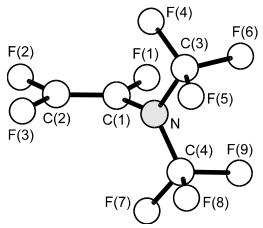


r_a	Å [a])
C(1)=C(2)	1.320 [b])
N–C(1)	1.386(6) [c])
N–C(3,4)	1.427(5) [c])
C(3,4)–F	1.328(2) [c])
C(1)–F(1)	1.339(2) [c])
C(2)–F(2,3)	1.304(2) [c])

θ_a	deg [a])
C(2)=C(1)–N	119.5(15)
C(1)–N–C(3)	117.6(12) [c])
C(1)–N–C(4)	119.4(12) [c])
C(3)–N–C(4)	117.8(10)
F–C–F (mean)	110.8(6)
C(2)=C(1)–F(1)	120.7(18) [c])
C(1)=C(2)–F(2,3)	125.0(18) [c])
$\sum\alpha$(N) [d])	354.8(6)
C(4)–N–C(3)–F(4)	164(9)
C(3)–N–C(4)–F(7)	174(11)
C=C–N–lp [e])	2(5)

Local C_{3v} symmetry was assumed for the CF_3 groups. The fluorovinyl group was assumed to be planar.
The nozzle was at room temperature.

[a]) Three times the estimated standard errors.
[b]) Estimated according to the results of B3LYP/6-31G* calculations.
[c]) Differences in the N–C and C–F bond lengths and in the C–N–C and C=C–F bond angles were assumed at the values from B3LYP/6-31G* calculations.
[d]) Sum of the angles at the N atom.
[e]) lp is the lone pair axis of the nitrogen atom.



Trautner, F., Abe, T., Oberhammer, H.: J. Am. Chem. Soc. **123** (2001) 2865.