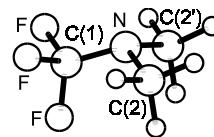


**1252 C<sub>3</sub>H<sub>6</sub>F<sub>3</sub>N**ED, *ab initio* calculations  
(HF/3-21G\*)

$r_a$	Å <sup>a)</sup>
C–F	1.351(4)
N–C(1)	1.383(16)
N–C(2)	1.481(10)
C–H	1.091(8)

**1,1,1-Trifluoro-*N,N*-dimethylmethanamine***N,N*-Dimethyltrifluoromethylamine

$\theta_\alpha$	deg <sup>a)</sup>
C(2)–N–C(2')	113.0(27)
C(1)–N–C(2)	111.9(9)
F–C–F	106.1(5)
H–C–H	109.0 <sup>b)</sup>
$\tau$ (CF <sub>3</sub> ) <sup>c)</sup>	3.6(13)

**C<sub>s</sub>**F<sub>3</sub>C–N(CH<sub>3</sub>)<sub>2</sub>

Overall C<sub>s</sub> symmetry with the two methyl groups exactly staggered to the opposite N–C(2) bond and local C<sub>3v</sub> symmetry for the CH<sub>3</sub> and CF<sub>3</sub> groups were assumed. The nozzle was at room temperature.

<sup>a)</sup> Three times the estimated standard errors including the scale error.

<sup>b)</sup> Fixed at *ab initio* value.

<sup>c)</sup> Tilt angle between the C<sub>3</sub> axis of the CF<sub>3</sub> group and the N–C bond direction towards the nitrogen lone pair.

Jin, A., Zhu, X.-L., Kirchmeier, R.L., Shreeve, J.M., Patel, N.R., Oberhammer, H.: J. Mol. Struct. **323** (1994) 129.