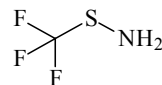


**99 CH<sub>2</sub>F<sub>3</sub>NS**ED, MW, DFT  
calculations**1,1,1-Trifluoromethanesulfenamide****C<sub>s</sub> (*syn*)****C<sub>s</sub> (*anti*)**

$r_z$	Å <sup>a)</sup>	$\theta_z$	deg <sup>a)</sup>
S–C	1.836(5)	C–S–N	101.8(8)
C–F (mean)	1.331(2)	F–C–F (mean)	108.4(3)
$\Delta(\text{C–F})$ <sup>b)</sup>	0.007(3) <sup>c)</sup>	$\Delta(\text{F–C–F})$ <sup>d)</sup>	1.7(2)
C–F(1)	1.326(4)	F(1)–C–F(2)	108.9(4)
C–F(2)	1.334(3)	F(2)–C–F(2')	107.2(4)
S–N	1.673(5)	tilt(CF <sub>3</sub> ) <sup>e)</sup>	2.0(13)
N–H	1.012(8)	S–N–H	115.3(20)
		H–N–H'	111.3 <sup>f)</sup>



The molecule was found to exist as a mixture of *anti* and *syn* conformers. The energy difference  $\Delta E = E(\text{syn}) - E(\text{anti}) = 1.1(1) \text{ kcal mol}^{-1}$  was derived from the relative intensities of transition in the MW spectra and dipole moments. This experimental value was reproduced reasonably well by B3PW91/6-31G\* calculations ( $\Delta E = E(\text{syn}) - E(\text{anti}) = 0.8 \text{ kcal mol}^{-1}$ ).

The nozzle was at room temperature.

<sup>a)</sup> Twice the estimated standard errors.

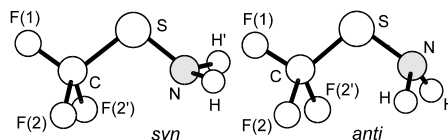
<sup>b)</sup>  $[\text{C–F}(2)] - [\text{C–F}(1)]$ .

<sup>c)</sup> Not refined, but varied within the estimated uncertainty.

<sup>d)</sup>  $[\text{F}(1)\text{–C–F}(2)] - [\text{F}(2)\text{–C–F}(2')]$ .

<sup>e)</sup> Tilt angle of the CF<sub>3</sub> group in the CSN plane away from the nitrogen atom.

<sup>f)</sup> Assumed at the value from B3PW91/6-31G\* calculations.



Asimus, M., Schühle, S., Christen, D., Møllendal, H., Della Vedova, C.O., Lieb, M., Oberhammer, H.: J. Mol. Struct. **485-486** (1999) 163.