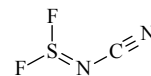


**35**      **CF<sub>2</sub>N<sub>2</sub>S**ED, *ab initio* and  
DFT calculations**Sulfur cyanamide difluoride**

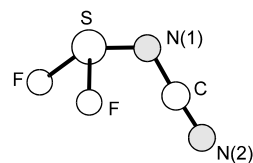
(Cyanoimido)difluorosulfur

**C<sub>s</sub>**

$r_a$	Å <sup>a)</sup>	$\theta_a$	deg <sup>a)</sup>
C≡N(2)	1.167(3)	S=N–C	126.2(15)
N(1)–C	1.368(4)	N=S–F	108.8(8)
S=N	1.484(3)	F–S–F	90.5(3)
S–F	1.593(2)	N–C≡N	179.0(28)

The molecule was found to exist as a *syn* conformer with the C≡N bond in the *syn* position with respect to the bisector of the F–S–F angle. According to the results of HF, MP2 and B3LYP calculations, the energy difference between the *anti* and *syn* conformers is more than 5 kcal mol<sup>−1</sup>.

The nozzle was at room temperature.



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

Alvaréz, R.S.M., Cutin, E.H., Della Vedova, C.O., Mews, R., Haist, R., Oberhammer, H.: Inorg. Chem. **40** (2001) 5188.