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CFNOS

**Sulfinyl cyanide fluoride**

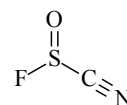
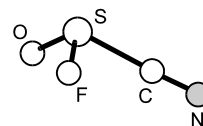
Thionyl cyanide fluoride

Cyanosulfurous fluoride

C<sub>1</sub>

$r_a$	$\text{\AA}^a$
C≡N	1.150(3)
S=O	1.432(2)
S–F	1.598(3)
S–C	1.783(3)

$\theta_a$	deg <sup>a</sup>
F–S=O	104.9(4)
C–S=O	105.3(5)
F–S–C	93.9(4)
S–C≡N <sup>b</sup>	176(4)



The experimental bond lengths were reproduced well by values from HF/3-21G\*, HF/6-31G\* and MP2/6-31G\* calculations. The bond angles were reproduced by these methods within *ca.*  $\pm 3^\circ$ .

The nozzle was probably at room temperature.

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

<sup>b</sup>) Bent towards the S lone pair.

Mack, H.-G., Oberhammer, H., Jacobs, J., Kronberg, M., Willner, H.: Inorg. Chem. **35** (1996) 806.