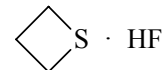
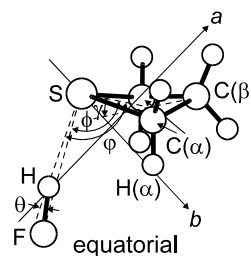
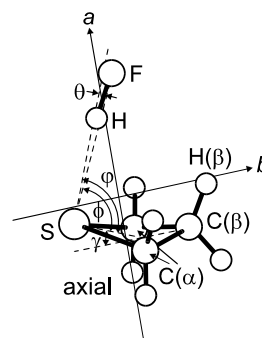


420
MW $\text{C}_3\text{H}_7\text{FS}$ **Thietane – hydrogen fluoride (1/1)**
(weakly bound complex) C_s
(large-amplitude motion)
(effective symmetry class)

r_0	$\text{\AA}^a)$		θ_0	$\text{deg}^a)$	
	axial	equatorial		axial	equatorial
S–C(α)	1.833(6)	1.833(17)	C(α)–S–C(α)	76.8(4)	76.8(9)
C(α)–C(β)	1.546(7)	1.56(2)	C(β)–C(α)–S	91.2(3)	91.8(9)
C(α)...C(α)	2.277(5)	2.276(5)	C(α)–C(β)–C(α)	94.9(5)	93.6(17)
F...S	3.094(2)	3.067(14)	H–C–H	108 ^{b)}	108 ^{b)}
F...H(α)		3.09(3)	$\gamma^c)^d)$	25.4(4)	25(2)
F...H(β)	2.97(2)		$\phi^d)^e)$	88.82(16)	89.8(3)
S...H	2.17(4)	2.16(6)	$\phi^d)^f)$	91.1(15)	93(3)
C–H	1.09 ^{b)}	1.09 ^{b)}	$\theta^d)^g)$	8(4)	12(6)

The axial conformer has been found to be the most stable; the intensity ratio of the two conformers (axial/equatorial) was approximately 7:1. This conformational preference has been explained in the context of a delicate balance between primary and secondary hydrogen bonds. Both conformers have C_s symmetry with the hydrogen fluoride located in the molecular symmetry plane of trimethylene sulfide, which is puckered at a similar angle to that found for the bare ring.



^{a)} Estimated standard errors.

^{b)} Assumed. A local C_{2v} symmetry was also assumed for the CH_2 groups.

^{c)} Ring puckering angle.

^{d)} See figure for the definition.

^{e)} Angle between the line bisecting the C–S–C angle and the S...F internuclear line.

^{f)} Angle between the line bisecting the C–S–C angle and the S...H hydrogen bond.

^{g)} Angle of deviation of the S...H–F fragment from collinearity.

Sanz, M.E., López, J.C., Alonso, J.L.: Chem. Eur. J. **8** (2002) 4265.