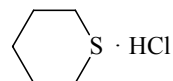


669
MW $C_5H_{11}ClS$

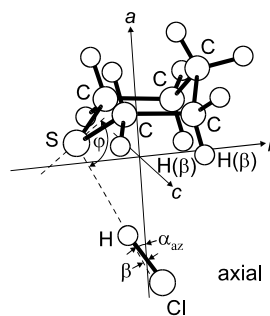
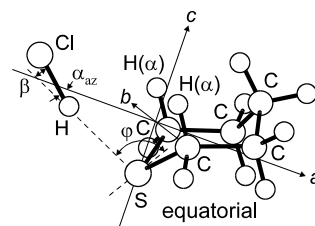
Tetrahydro-2*H*-thiopyran – hydrogen chloride (1/1) C_s (axial)
 (weakly bound complex) C_s (equatorial)
 (effective symmetry class)
 (large-amplitude motion)

r_0	\AA^a	
	axial	equatorial
S...H ^{b)}	2.35(8)	2.19(5)
S...Cl	3.63(4)	3.44(2)

θ_0	deg ^{a)}	
	axial	equatorial
$\phi^c)$	98.3(11)	91.8(9)
$\varphi^d)$	100(2)	98.1(10)
$\beta^e)$	6(3)	17.2(2)
$\alpha_{az}^e) ^f)$	32.9(17)	39.843(36)



Interpretation of the rotational constants led to the conclusion that the observed complexes have C_s symmetry with the hydrogen chloride pointing to the domain of axial or equatorial lone pairs at the sulfur atom. The equatorial form has been found to be the most stable.



^{a)} Estimated standard errors.

^{b)} Hydrogen atom of the HCl subunit.

^{c)} Angle between the S...Cl line and the line bisecting the C–S–C angle.

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

^{e)} See figure for the definition.

^{f)} Values corresponding to the parent isotopic species.

Sanz, M.E., López, J.C., Alonso, J.L: Chem. Eur. J. **5** (1999) 3293.