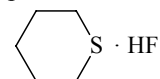
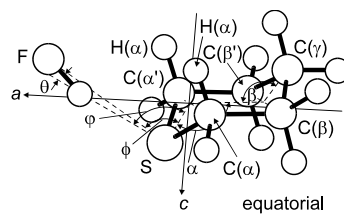


671  
MW $\text{C}_5\text{H}_{11}\text{FS}$ **Tetrahydro-2*H*-thiopyran – hydrogen fluoride (1/1)**  $\text{C}_s$  (axial)  
(weakly bound complex)  $\text{C}_s$  (equatorial)(effective symmetry class)  
(large-amplitude motion)

$r_0$	$\text{\AA}^{\text{a}}$		$\theta_0$	$\text{deg}^{\text{a}}$	
	axial	equatorial		axial	equatorial
F...S	3.114(4)	3.10(2)	$\phi^{\text{b}}$	101.8(5)	91(2)
H...S	2.19(1)	2.18(2)	$\phi^{\text{b}}$	101.8(5)	95(4)
F...H( $\alpha$ )		3.15(3)	$\theta^{\text{b}}$	0.0 $^{\text{c}}$	11(10)
F...H( $\beta$ )	2.81(2)		C( $\alpha$ )–S–C( $\alpha'$ )	98.6(5)	97(2)
S–C( $\alpha$ )	1.812(8)	1.81(3)	S–C( $\alpha$ )–C( $\beta$ )	112.9(6)	112(2)
C( $\alpha$ )–C( $\beta$ )	1.524(9)	1.52(2)	C( $\alpha$ )–C( $\beta$ )–C( $\gamma$ )	112.1(9)	112(1)
C( $\beta$ )–C( $\gamma$ )	1.52(1)	1.54(1)	C( $\beta$ )–C( $\gamma$ )–C( $\beta'$ )	112.3(8)	113(1)
C–H	1.095 $^{\text{c}}$	1.095 $^{\text{c}}$	H–C–H	108.5 $^{\text{c}}$	108.5 $^{\text{c}}$
			$\alpha^{\text{b}}$	132.0(7)	129(3)
			$\beta^{\text{b}}$	126(1)	127(2)

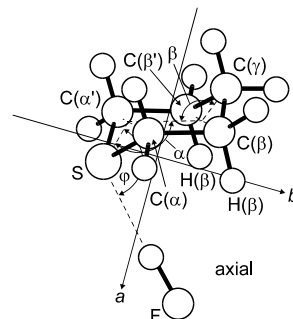
The axial form was found to be more stable. No equatorial-to-axial relaxation was observed when He or Ar was used as the carrier gas. No significant structural distortion of pentamethylene sulfide upon complexation was detected. Local  $\text{C}_{2v}$  symmetry was assumed around the C atoms.



<sup>a</sup>) Estimated standard errors.

<sup>b</sup>) See figure for the definition.

<sup>c</sup>) Assumed.



Blanco, S., Lesarri, A., López, J.C., Alonso, J.L.:  
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