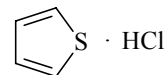
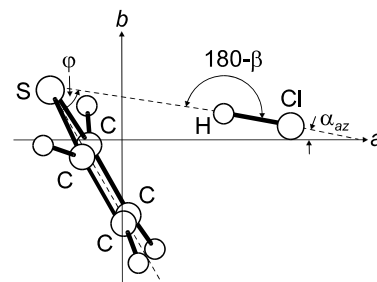


519  
MW $\text{C}_4\text{H}_5\text{ClS}$ **Thiophene – hydrogen chloride (1/1)**  
(weakly bound complex) $\text{C}_s$   
(effective symmetry class)  
(large-amplitude motion)

$r_0$	$\text{\AA}$	$\theta_0$	deg
S...H	2.7474(29)	$\varphi^c$	64.53(16)
cm...Cl <sup>a)</sup>	3.693(5) <sup>b)</sup>	$\beta^c$	0.97(64)
		$\alpha_{az}^c$ <sup>d)</sup>	12.46(43)
		S...cm...Cl <sup>a)</sup>	98.96(50) <sup>b)</sup>



Interpretation of the spectroscopic constants led to the conclusion that the observed complex has  $\text{C}_s$  symmetry, with the Cl atom of HCl lying almost directly above the center of mass of the thiophene ring but with the H atom of HCl pointing at the  $\pi$ -electron density near to the S atom. The S...H–Cl nuclei are almost collinear [ $\beta = 0.9(6)^\circ$ ], but the relatively large distance  $r(\text{S}...\text{H}) = 2.7474(29) \text{ \AA}$  indicates that the S...H interaction is weak.



<sup>a)</sup> cm denotes the center of mass of thiophene.

<sup>b)</sup> Uncertainties were not estimated in the original paper.

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

<sup>d)</sup> For  $\text{C}_4\text{H}_4^{32}\text{S}\cdot\text{H}^{35}\text{Cl}$ .

Cooke, S.A., Corlett, G.K., Legon, A.C.: J. Chem. Soc., Faraday Trans. **94** (1998) 1565.