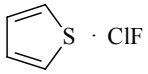
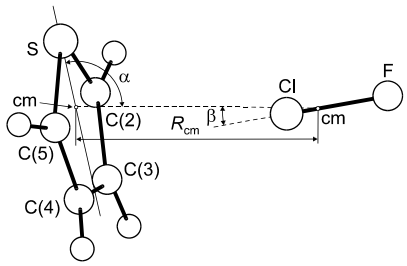
507 **C_4H_4ClFS** **Thiophene – chlorine fluoride (1/1)** **C_1**
MW (weakly bound complex) (effective symmetry class)
(large-amplitude motion)



r_0	Å [a])
R_{cm}	3.7690(20)

θ_0	deg [a])			
	1 [b])	2 [b])	3 [b])	4 [b])
α [c])	103.40(20)	76.60(20)	76.52(20)	103.48(20)
β [c])	–19.3(3)	19.3(3)	–21.3(3)	21.3(3)
γ [d])	66.87(30)	113.13(30)	66.89(30)	113.11(30)
δ [e])	58.5(3)	58.5(3)	67.3(3)	67.3(3)

The geometry of the present complex was determined by using the direction cosines θ_{az}, θ_{bz} and θ_{cz} (z is the ClF axis), determined by diagonalization of the Cl nuclear quadrupole coupling tensor, in combination with principal moments of inertia. Four geometries of thiophene · ClF are consistent with the observed quantities, but each has ClF interacting with the π-electron system on one face of the thiophene ring.



[a]) Uncertainties were not estimated in the original paper.
[b]) Four possible structures.
[c]) See figure for the definition.
[d]) Dihedral angle cm(ClF)...cm(C_4H_4S)...S–C(2).
[e]) Dihedral angle Cl–cm(ClF)...cm(C_4H_4S)...S.

Cooke, S.A., Holloway, J.H., Legon, A.C.: Chem. Phys. Lett. **298** (1998) 151.