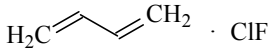
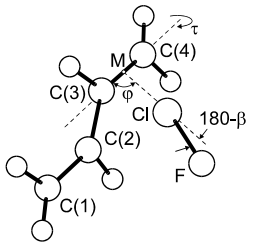
526 **C_4H_6ClF** **1,3-Butadiene – chlorine fluoride (1/1)** **C_1**
MW (weakly bound complex) (large-amplitude motion)



r_0	Å
M...Cl [a])	2.736(4)

θ_0	deg
φ [b])	95.0(2)
β [b])	177.4(10)
τ [b]) [c])	90 [d])

A detailed interpretation of the observed spectroscopic constants led to the conclusion that the Cl end of the ClF molecule interacts with the C(3)=C(4) π bond of 1,3-butadiene to give a complex in which the ClF molecule is perpendicular to the plane of 1,3-butadiene. The intermolecular stretching force constant is 6.21 N m^{-1}.



[a]) M denotes the mid-point of the C(3)=C(4) bond.
[b]) See figure for the definition.
[c]) $\tau = 90°$ defines the geometry in which ClF is perpendicular to the plane of 1,3-butadiene.
[d]) Assumed.

Cooke, S.A., Holloway, J.H., Legon, A.C.: J. Chem. Soc., Faraday Trans. **93** (1997) 2361.