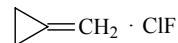


527
MW

 $\text{C}_4\text{H}_6\text{ClF}$
Methylenecyclopropane – chlorine fluoride (1/1)
(weakly bound complex)

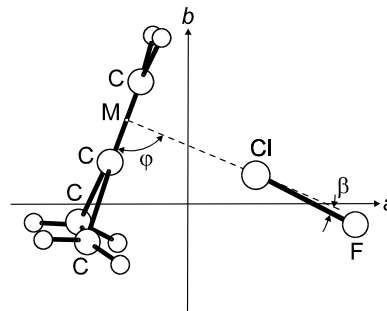
 C_s
(effective symmetry class)
(large-amplitude motion)


r_0	\AA	θ_0	deg
M...Cl ^{a)}	2.675(10)	φ ^{b)}	92.5(5)
		β ^{b)}	4.9(1)

The intermolecular force constant k_σ is 10.23 and 10.31 N m⁻¹ for the ³⁵Cl and ³⁷Cl species, respectively. The complex is a Mulliken outer one, which may be described formally as of the $b\pi.a\sigma$ type, *i.e.*, with the electrophilic end $\delta^+\text{Cl}$ of ClF interacting weakly with the π bond of methylenecyclopropane and with only electric charge redistribution within the ClF subunit.

^{a)} M denotes the center of the C=C bond.

^{b)} See figure for the definition.



Cooke, S.A., Holloway, J.H., Legon, A.C.: J. Chem. Soc., Faraday Trans. **93** (1997) 4253.