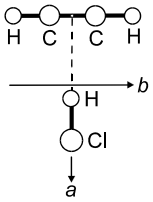
234 **C_2H_3Cl** **Ethyne – hydrogen chloride (1/1)** **C_{2v}**
IR, *ab initio* calculations (CCDS(T)/cc-pVTZ)
(weakly bound complex)
(effective symmetry class)
(large-amplitude motion)
HC≡CH · HCl

r_e	Å [a] [b])
C≡C	1.210(1)
C–H	1.064(1)
H–Cl	1.283(5)
Cl…π [c])	3.678(1)



[a]) Results of CCDS(T)/cc-pVTZ calculations were used for the structure determination, because they describe best the experimental monomer properties (geometries, energies and infrared harmonic frequencies).
[b]) Deviations upon complexation in parentheses.
[c]) Separation between the Cl atom and the center of the C≡C bond.

Carcabal, P., Broquier, M., Chevalier, M., Picard-Bersellini, A., Brenner, V., Millié, P.: J. Chem. Phys. **113** (2000) 4876.

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