

1585  
MW

**C<sub>4</sub>H<sub>5</sub>F**

**Vinylacetylene – hydrogen fluoride (1/1)**  
(weakly bound complex)

**C<sub>s</sub>**  
(effective symmetry class)  
H<sub>2</sub>C=CH–C≡CH · HF

$r_0$ [Å]	1 <sup>a)</sup>	1+2 <sup>a)</sup>	1 <sup>a)</sup>	1+2 <sup>a)</sup>
$R(\text{CC}\dots\text{F})$	3.0693(10)	3.0693(7)	3.0713(5)	3.0715(20) <sup>b)</sup>
$d$ <sup>c)</sup>	–	–	0.0035(8)	0.0039(30) <sup>b)</sup>
$\delta(\text{D–H})$ <sup>d)</sup>	–	–0.0015	–	–0.0015

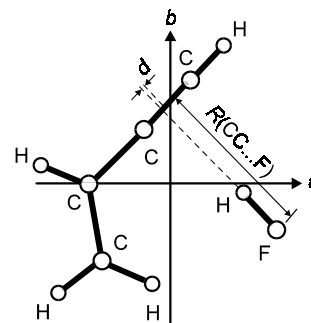
The HF molecule attaches preferentially to the triple bond in vinylacetylene, in a T-type configuration close to the C≡C bisector. As for the quasiplanarity (*i.e.*, the double-minimum intermolecular potential) in equilibrium, an estimated limit of 9° is placed on the departure from planarity.

<sup>a)</sup> 1: H<sub>2</sub>C=CH–C≡CH · HF; 2: H<sub>2</sub>C=CH–C≡CH · DF.

<sup>b)</sup> Uncertainty is larger than those of the original data.

<sup>c)</sup> Displacement of the HF axis from the midpoint of the C≡C bond in the direction of C<sub>2</sub>.

<sup>d)</sup>  $\delta(\text{D–H}) = [R(\text{CC}\dots\text{F})]_{\text{D}} - [R(\text{CC}\dots\text{F})]_{\text{H}}$ .



Kisiel, Z., Fowler, P.W., Legon, A.C.: Chem. Phys. Lett. **176** (1991) 446.