

1619
MW

C_4H_6

Ethylene – acetylene (1/1)
(weakly bound complex)

C_{2v}
(effective symmetry class)
 $H_2C=CH_2 \cdot HC\equiv CH$
 $H_2C=CH_2 \cdot DC\equiv CD$
 $H_2C=CH_2 \cdot DC\equiv CH$
 $DHC=CHD \cdot HC\equiv CH$

Isotopic species	$r_0(R_{cm})$ [Å]	$r_0(H)$ [Å] ^{a)}
$H_2C=CH_2 \cdot HCCH$	4.443	2.78
$H_2C=CH_2 \cdot DCCD$	4.442	2.78
$H_2C=CH_2 \cdot DCCH$	4.380	2.78
$t\text{-}DHC=CDH \cdot HCCH$	4.441	2.78
	4.442(2) (average)	2.780(2) (average)

This complex has a C_{2v} structure in which the HCCH unit hydrogen-bonds to ethylene π cloud, with the HCCH axis normal to the plane of the ethylene. Tunneling splitting due to the hindered internal rotation of the ethylene unit about its C=C bond led to a barrier of 240 cm^{-1} .

^{a)} Hydrogen-bond length.

Fraser, G.T., Lovas, F.J., Suenram, R.D., Gillies, J.Z., Gillies, C.W.: Chem. Phys. **163** (1992) 91.

