

230 **C₂H₃⁺** **Protonated acetylene** **C_{2v}**
 MW Ethenylium

(effective symmetry class)
 (large-amplitude motion)
 non-classical form: HC(H⁺)CH
 classical form:



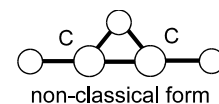
r_0	Å ^{a)}	θ_0	deg ^{a)}
C–C	$1.246 - 0.019\cos[\pi(\eta+1)]$	ζ	$30(\eta + 2)$
C(1)–H(1)	$1.116 - 0.011\eta + 0.169\eta^2$	α ^{b)}	$120.420 + 72.425\eta + 13.745\eta^2$
C(1)–H(2)	$1.116 + 0.053\eta + 0.033\eta^2$	β ^{b)}	$180.00 - 42.060\eta - 42.960\eta^2$
C(2)–H(3)	$1.098 - 0.002\eta - 0.004\eta^2$	γ ^{b)}	$119.200 - 7.375\eta - 7.476\eta^2$

An internal-axis-method-like approach was applied to obtain crucial information on the proton trajectories along the tunneling path. The path coordinate η was defined to be equal to -1 at configuration 1 and $+1$ at configuration 2. The six configurations $n = 1 \sim 6$ were represented by the vibrational wavefunctions: $\psi_n(\zeta) = \exp\{-a[\zeta - (2n - 1)\pi/6]^2\}$.

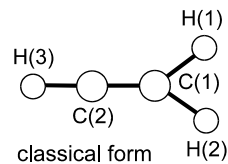
^{a)} Uncertainties were not estimated in the original paper.

Because the analysis is based on a special model for internal motion, it is quite difficult to evaluate uncertainties for coefficients of seven structural parameters.

^{b)} The angles α , β , and γ were defined according to Lindh, R., Roos, B.D., Kraemer, W.P.: Chem. Phys. Lett. **139** (1987) 7, namely $\alpha = \text{H}(1)\text{--C}(1)\text{--C}(2)$, $\beta = \text{C}(1)\text{--C}(2)\text{--H}(3)$, and $\gamma = \text{H}(1)\text{--C}(1)\text{--H}(2)$.



non-classical form



classical form

Cordonnier, M., Coudert, L.H.: J. Mol. Spectrosc. **178** (1996) 59.

See also: Hougen, J.T.: J. Mol. Spectrosc. **123** (1987) 197.

Crofton, M.W., Jagod, M.-F., Rehffuss, B.D., Oka, T.: J. Chem. Phys. **91** (1989) 5139.

Bogey, M., Bolvin, H., Cordonnier, M., Demuynck, C., Destombes, J.L., Escribano, R.,

Gomez, P.C.: Can. J. Phys. **72** (1994) 967.