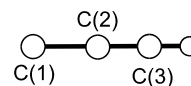


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MW**C₃H****2-Propynylidyne****C_{∞v}**
CC≡CH

r_s	Å ^{a)} ^{b)}	Å ^{b)} ^{c)}
C(1)–C(2)	1.3263(1)	1.3213(3)
C(2)≡C(3)	1.2539(2)	1.2607(3)
C(3)–H	1.0171(1)	1.0040(2)



Atom	z_s [Å] ^{a)}	z_s [Å] ^{c)}
C(1)	–1.36468	–1.36329
C(2)	–0.03836	–0.04203
C(3)	1.21552	1.21864
H	2.23266	2.22266

The short C–H distance is interpreted in terms of a large-amplitude motion of the ν_4 mode, whose vibrational energy is very low due to the Renner-Teller effect. *Ab initio* calculations were carried out, and the structure in which the HCC angle is bent was found to be slightly more stable than the linear structure.

^{a)} $^2\Pi_r$ ground vibronic state.

^{b)} Three times the estimated standard errors.

^{c)} $^2\Sigma^u$ low-lying excited vibronic state of the ν_4 (HCC bending) vibrational mode.

Kanada, M., Yamamoto, S., Saito, S., Osamura, Y.: J. Chem. Phys. **104** (1996) 2192.