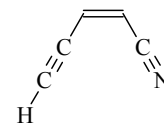


624 C_5H_3N

(2Z)-2-Penten-4-ynenitrile

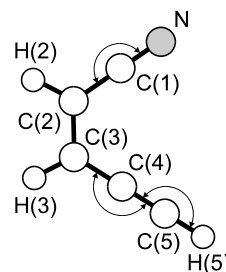
 C_s MW, *ab initio*
calculations

r_0	\AA^a	θ_0	deg^a
N≡C(1)	1.161(5)	N≡C(1)–C(2)	178.6(5)
C(1)–C(2)	1.428(5)	C(1)–C(2)=C(3)	122.6(5)
C(2)=C(3)	1.343(5)	C(2)=C(3)–C(4)	123.9(5)
C(3)–C(4)	1.418(5)	C(3)–C(4)≡C(5)	179.5(5)
C(4)≡C(5)	1.212(5)	H–C(2)=C(3)	122.9(7)
C(2)–H	1.101(7)	H–C(3)–C(4)	115.8(7)
C(3)–H	1.097(7)	C(4)≡C(5)–H	179.3(7)
C(5)–H	1.054(7)	N≡C(1)–C(2)=C(3) ^{b)}	180.0
		C(2)=C(3)–C(4)≡C(5) ^{b)}	180.0
		C(3)–C(4)≡C(5)–H ^{b)}	180.0

r_s	\AA^a	θ_s	deg^a
N≡C(1)	1.151(5)	N≡C(1)–C(2)	178.0(5)
C(1)–C(2)	1.437(5)	C(1)–C(2)=C(3)	122.3(5)
C(2)=C(3)	1.343(5)	C(2)=C(3)–C(4)	123.2(5)
C(3)–C(4)	1.442(5)	C(3)–C(4)≡C(5)	178.0(5)
C(4)≡C(5)	1.188(5)	H–C(2)=C(3)	122.8(7)
C(2)–H	1.101(7)	H–C(3)–C(4)	116.5(7)
C(3)–H	1.097(7)	C(4)≡C(5)–H	178.4(7)
C(5)–H	1.057(7)	N≡C(1)–C(2)=C(3) ^{b)}	180.0
		C(2)=C(3)–C(4)≡C(5) ^{b)}	180.0
		C(3)–C(4)≡C(5)–H ^{b)}	180.0

r_e	\AA^c	θ_e	deg^c
N≡C(1)	1.158(5)	N≡C(1)–C(2)	178.7(5)
C(1)–C(2)	1.427(5)	C(1)–C(2)=C(3)	122.6(5)
C(2)=C(3)	1.345(5)	C(2)=C(3)–C(4)	123.9(5)
C(3)–C(4)	1.420(5)	C(3)–C(4)≡C(5)	179.5(5)
C(4)≡C(5)	1.207(5)	H–C(2)=C(3)	119.5(5)
C(2)–H	1.072(5)	H–C(3)–C(4)	117.9(5)
C(3)–H	1.079(5)	C(4)≡C(5)–H	179.2(5)
C(5)–H	1.062(5)	N≡C(1)–C(2)=C(3) ^{b)}	180.0
		C(2)=C(3)–C(4)≡C(5) ^{b)}	180.0
		C(3)–C(4)≡C(5)–H ^{b)}	180.0

Atom	a_0 [\AA]	b_0 [\AA]
N	–2.06734	1.07466
C(1)	–1.43222	0.10329
C(2)	–0.67997	–1.10994
C(3)	0.66321	–1.12792
C(4)	1.46950	0.03789
C(5)	2.16714	1.02833
H(2)	–1.29000	–2.02668
H(3)	1.20321	–2.08241
H(5)	2.76295	1.89810



- ^{a)} Uncertainties were not estimated in the original paper.
- ^{b)} 180.0° means that the four atoms are on the same plane.
- ^{c)} Vibration-rotation constants were computed by an *ab initio* SDQ-MBPT(4)/DZP method.

Halter, R.J., Fimmen, R.L., McMahon, R.J., Peebles, S.A., Kuczkowski, R.L., Stanton, J.F.:
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