

1701
MW

C₄H₇N

3,4-Dihydro-2*H*-pyrrole
1-Pyrroline

C₁

r_0	Å	θ_0	deg
C(5)–N	1.466 ^{a)}	C(3)–C(4)–C(5)	103.9 ^{a)}
C(3)–C(4)	1.545 ^{a)}	H–C–H (average)	107.4 ^{a)}
C(2)=N	1.252 ^{a)}	N=C(2)–C(3)	117.1 ^{a)}
C(2)–H	1.074 ^{a)}	N=C(2)–H	120.9 ^{a)}
C(4)–C(5)	1.552 ^{a)}	N=C(2)–H	116.2(1)
C(2)–C(3)	1.509 ^{a)}	φ ^{b)}	22.9(2)
C–H (average)	1.082 ^{a)}		
C(2)=N	1.306(2)		

^{a)} *Ab initio* value.

^{b)} Equilibrium puckering angle. Uncertainty was not estimated in the original paper.

Edwards, G.B., Yamanouchi, K., Kuchitsu, K., Sugie, M., Takeo, H., Matsumura, C.,
Ogawa, K., Takeuchi, Y.: J. Mol. Spectrosc. **111** (1985) 301.

