

1593
MW

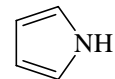
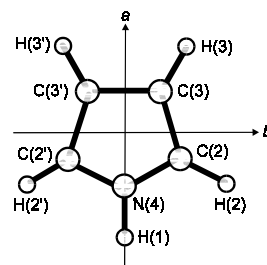
C₄H₅N

Pyrrole

C_{2v}

r_s	Å	θ_s	deg
N–C	1.370(5)	C–N–C	109.8(3)
C(2)=C(3)	1.382(5)	N–C=C	107.7(3)
C(3)–C(3')	1.417(5)	C(2)=C(3)–C(3')	107.4(3)
N–H	0.996(10)	N–C(2)–H	121.5(10)
C(2)–H	1.076(10)	H–C(3)–C(3')	127.1(10)
C(3)–H	1.077(10)		

Atom	a_s [Å]	b_s [Å]
N	–1.12220	0.0
C(2,2')	–0.33395	±1.12111
C(3,3')	0.98522	±0.70837
H(1)	–2.11771	0.0
H(2,2')	–0.7605	±2.1089
H(3,3')	1.8443	±1.3578



The molecule is planar.

Nygaard, L., Nielsen, J.T., Kirchheiner, J., Maltesen, G., Rastrup-Andersen, J., Sørensen, G.O.:
J. Mol. Struct. **3** (1969) 491.

See also:

Bak, B., Christensen, D., Hansen, L., Rastrup-Andersen, J.: J. Chem. Phys. **24** (1956) 720.