

1153
MW

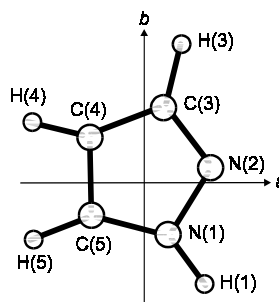
C₃H₄N₂

Pyrazole

C_s

r_s	Å	θ_s	deg
N(1)–N(2)	1.351(10)	N(1)–N(2)=C(3)	104.1(3)
N(2)=C(3)	1.332(5)	N(2)=C(3)–C(4)	112.0(3)
C(3)–C(4)	1.417(5)	C(3)–C(4)=C(5)	104.5(3)
C(4)=C(5)	1.374(5)	C(4)=C(5)–N(1)	106.4(3)
C(5)–N(1)	1.360(5)	C(5)–N(1)–N(2)	113.0(3)
N(1)–H(1)	1.002(10)	N(2)=C(3)–H(3)	119.3(5)
C(3)–H(3)	1.083(10)	C(3)–C(4)–H(4)	127.9(5)
C(4)–H(4)	1.080(10)	N(1)–C(5)–H(5)	121.4(5)
C(5)–H(5)	1.082(10)	N(2)–N(1)–H(1)	118.4(5)

Atom	a_s [Å]	b_s [Å]
N(1)	0.39883	–0.9997
N(2)	1.17514	0.1033
C(3)	0.30582	1.1106
C(4)	–1.03436	0.6530
C(5)	–0.93022	–0.7156
H(1)	0.8435	–1.8930
H(3)	0.6728	2.1246
H(4)	–1.9340	1.2426
H(5)	–1.6724	–1.4965



The molecule is planar.

Nygaard, L., Christen, D., Nielsen, J.T., Pedersen, E.J., Snerling, O., Vestergaard, E., Sørensen, G.O.: J. Mol. Struct. **22** (1974) 401.

