

510
MW $C_4H_4N_2$

Pyrimidine

 C_{2v} 

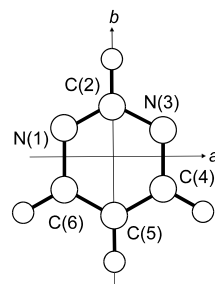
r_0	\AA
N–C(2)	1.338(4)
N–C(4)	1.339(5)
C–C	1.393(4)
C–H	1.089 ^a)

θ_0	deg
N–C–N	127.4(4)
C–N–C	115.7(4)
N–C–C	122.3(4)
C–C–C	116.6(3)
C(5)–C(4)–H	121 ^a)

r_s	\AA
N–C(2)	1.337(2)
N–C(4)	1.332(3)
C–C	1.393(2)

θ_s	deg
N–C–N	127.2(3)
C–N–C	115.8(3)
N–C–C	122.4(3)
C–C–C	116.4(2)

Atom	$ a_s [\text{\AA}]$	$ b_s [\text{\AA}]$
C(2)	0.0	1.2791
C(4)	1.1843	0.6468
C(5)	0.0	1.3804
N	1.1982	0.6848

^a) Assumed.

Kisiel, Z., Pszczółkowski, L., López, J.C., Alonso, J.L., Marris, A., Caminati, W.: J. Mol. Spectrosc. **195** (1999) 332.

[II/25C \(3, 1553\)](#)