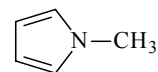


642 **C₅H₇N**
ED, MW, *ab initio*
calculations

1-Methyl-1*H*-pyrrole
N-Methylpyrrole

C_s assumed



r_z	\AA^a	θ_z	deg^a
N–C(2)	1.372(6)	C(2)–N–C(5)	109.3(9)
N–C(6)	1.452(7)	N–C(2)=C(3)	108.2(7)
C(2)=C(3)	1.383(9)	C(2)=C(3)–C(4)	107.1(4)
C(3)–C(4)	1.425(11)	H–C(2)–N	117.7(29)
C(2)–H	1.079(4) ^b	H–C(2)=C(3)	134.2(32)
C(3)–H	1.081(4) ^b	H–C(3)=C(2)	124.0(42)
C(6)–H	1.100(4) ^c	H–C(3)–C(4)	128.9(44)
		H–C(6)–H	109.1(3)
		H(1)–C(6)–N	109.9(3)

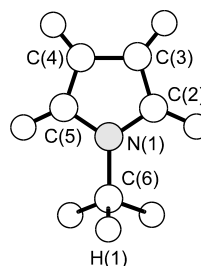
The molecular structure was reinvestigated using ED intensities from [1] and rotational constants of ¹³C- and ¹⁵N-substituted species from [2]. Local C_{2v} symmetry was assumed for the C(6)–ring fragment and C_{3v} for the CH₃ group. The methyl torsion was treated as a large-amplitude motion. The molecular symmetry in the equilibrium structure was assumed to be C_s, as shown in the figure.

The temperature of the ED measurements was 28 °C.

^a) Three times the estimated standard errors.

^b) All $r_g(\text{C–H})$ bond lengths in the ring were assumed to be equal.

^c) Difference between $r_g[\text{C–H}(\text{methyl})]$ and $r_g[\text{C–H}(\text{ring})]$ was assumed at the value from HF/6-31G* calculations.



Takeuchi, H., Inoue, K., Enmi, J., Hamada, T., Shibuya, T., Konaka, S.: J. Mol. Struct. **567-568** (2001) 107.

[1] Kurai, N., Takeuchi, H., Konaka, S.: J. Mol. Struct. **318** (1994) 143.

[2] Huber, S., Ha, T.-K., Bauder, A.: J. Mol. Struct. **413-414** (1997) 93.

MW

G₁₂

r_s	\AA^a	θ_s	deg^a
N–C(2)	1.361(3)	C(2)–N–C(6)	124.8(3)
C(2)–	1.393(3)	C(2)–N–C(5)	110.5(3)
C(3)			
C(3)–	1.422(3)	C(3)–C(2)–N	107.7(3)
C(4)			
N–C(6)	1.452(3)	C(4)–C(3)–C(2)	107.0(3)
N...C(3)	2.228(3)		

Atom	$a_s [\text{\AA}]$	$b_s [\text{\AA}]$
N	0.6566	0.0
C(2),C(5)	−0.112	±1.1181
C(3),C(4)	−1.4512	±0.7109
C(6)	2.10824	0.0

All rotational transitions were found to be split into A–E doublets because of the internal rotation of the methyl group. The potential barrier was determined to be $V_6 = 67.8021 \text{ cm}^{-1}$.

^{a)} Uncertainties were not estimated in the original paper.

Huber, S., Ha, T.-K., Bauder, A.: J. Mol. Struct. **413-414** (1997) 93.

Huber, S., Makarewicz, J., Bauder, A.: Mol. Phys. **95** (1998) 1021.

[II/25D \(3, 1980\)](#)