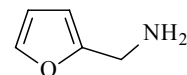


644 C₅H₇NOED, MW, *ab initio*
calculations**2-Furanmethanamine**

Furfurylamine

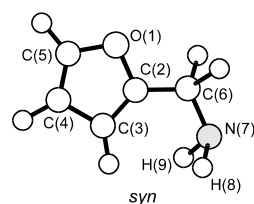
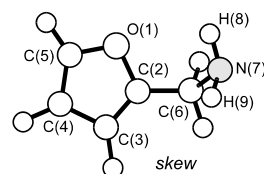
C₁ (*skew*)**C_s assumed (*syn*)**

r_g	Å ^{a)}	θ_α	deg ^{a)}
N–H ^{b)}	1.046(6)	C(2)–C(6)–N	114.1(6)
C–H ^{b)}	1.109(5)	C(6)–C(2)=C(3)	133.0(7)
C(2)–O	1.364(8)	C–O–C	108.4(10)
C(5)–O	1.359(8)	O–C(2)=C(3)	109.4(5)
C(2)=C(3)	1.370(8)	O–C(5)=C(4)	110.2(5)
C(4)=C(5)	1.366(8)	C(2)=C(3)–C(4)	106.3(2)
C(3)–C(4)	1.456(5)	C(5)=C(4)–C(3)	105.6(2)
C(2)–C(6)	1.493(8)	τ_1 ^{c)}	113.6(7)
C–N	1.474(7)	τ_2 ^{d)}	–56.8(22)



The molecule was found to exist as a mixture of *skew* (87(9)%) and *syn* (13(9)%) conformers. The furan ring was assumed to be planar. Differences in the symmetrically non-equivalent N–H, C–H, C–O, C=C distances, differences in the C=C–O bond angles and the bond angles to hydrogen atoms for the *skew* conformer were assumed at the values from MP2/6-311++G(2d,2p) calculations. Differences in the parameters between the *skew* and *syn* conformers were assumed at the values from MP2/6-311++G(2d,2p) calculations. The structural parameters are listed for the *skew* conformer.

The nozzle temperature was 25 °C.



^{a)} Twice the estimated standard errors including a systematic error.

^{b)} Average value.

^{c)} C(3)=C(2)–C(6)–N torsional angle, $\tau_1 = 0^\circ$ for the *syn* position.

^{d)} C–C–N–H(9) torsional angle, $\tau_2 = 0^\circ$ for the *syn* position.

Hagen, K., Postmyr, L.: J. Phys. Chem. A. **103** (1999) 11460.

[II/25D \(3, 1982\)](#)