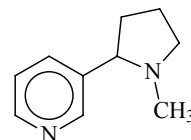


888 **C₁₀H₁₄N₂**
ED, *ab initio* and DFT
calculations

3-(1-Methyl-2-pyrrolidinyl)pyridine
Nicotine

C₁ (*eq-eq-syn*)
C₁ (*eq-eq-anti*)

r_g	Å ^{a)}	θ_α	deg ^{a)}
N–C (pyrrol) ^{b)}	1.462(4)	C(2)–N(1)–C(5)	108.4(15)
N(1)–C(m)	1.456(4)	N(1)–C(5)–C(4)	103.4 ^{c)}
N(1)–C(5)	1.464(4)	N(1)–C(2)–C(3)	101.3 ^{c)}
N(1)–C(2)	1.467(4)	C(3)–C(4)–C(5)	107.7(33)
C–C (pyrrol) ^{b)}	1.541(4)	C(2)–C(3)–C(4)	108.6 ^{c)}
C(4)–C(5)	1.534(4)	N(1)–C(2)–C(3')	116.8(10)
C(2)–C(3)	1.541(4)	C(3)–C(2)–C(3')	115.8(20)
C(3)–C(4)	1.547(4)	C(2')–N–C(6')	116.8(2)
C(2)–C(3')	1.502(4)	C(3')–C(2')–N	124.5(2)
C–N (pyrid) ^{b)}	1.345(2)	N–C(6')–C(5')	123.7(2)
C(2')–N	1.345(2)	C(2')–C(3')–C(4')	117.1 ^{c)}
C(6')–N	1.344(2)	C(4')–C(5')–C(6')	118.3 ^{c)}
C–C (pyrid) ^{b)}	1.397 ^{c)}	C(3')–C(4')–C(5')	119.5 ^{c)}
C(2')–C(3')	1.398(2)	H–C–H ^{b)}	111.9(41)
C(5')–C(6')	1.397(2)	N(1)–C(m)–H	113.5 ^{d)}
C(4')–C(5')	1.392(2)	α ^{e)}	45.7(25)
C(3')–C(4')	1.399(2)	ϕ ^{f)}	32.9(38)
C–H (pyrrol) ^{b)}	1.116(4)	C(3)–C(2)–C(3')–C(2')	–87.7(74)
C–H (pyrid) ^{b)}	1.106(4)	N(1)–C(2)–C(3')–C(2')	153.1 ^{c)}



According to the results of HF and MP2 calculations, the molecule was assumed to exist as a mixture of *eq-eq-syn* (67.4%) and *eq-eq-anti* (32.6%) conformers. The abbreviations correspond to the positions of the methyl group, pyridine ring and H–C(2)–C(3')–C(2'), respectively. Differences between the similar parameters of the conformers and in each conformer were assumed at the values from MP2/6-31G* calculations. The pyridine ring and the C(2)C(3)C(4)C(5) fragment were assumed to be planar. The structural parameters are listed for the *eq-eq-syn* conformer. The nozzle temperature was *ca.* 116 °C.

^{a)} Three times the estimated standard errors.

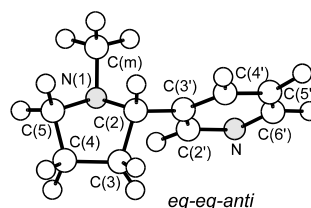
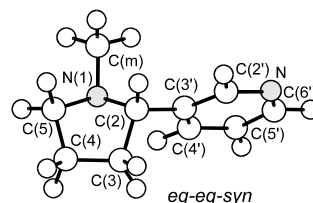
^{b)} Average value.

^{c)} Dependent parameter.

^{d)} Assumed at the value for *N*-methylpyrrolidine.

^{e)} Angle between the C(2)N(1)C(5) plane and N(1)–C(m) bond.

^{f)} Dihedral angle between the C(2)C(3)C(4)C(5) and C(2)N(1)C(5) planes.



Takeshima, T., Fukumoto, R., Egawa, T., Konaka, S.: J. Phys. Chem. A **106** (2002) 8734.