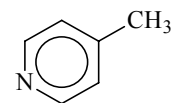


728 C₆H₇NED, MW, IR, *ab initio*
calculations**4-Methylpyridine***γ*-Picoline**C_s assumed**

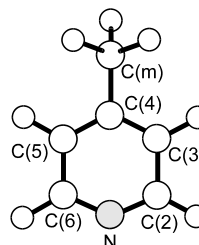
r_g	Å ^{a)}	θ_α	deg ^{a)}
C–N	1.347(5)	C(2)–C(3)–C(4)	119.9(4)
C(2)–C(3)	1.391(3)	C(3)–C(4)–C(5)	116.4(4)
C(3)–C(4)	1.395(3)	N–C(2)–C(3)	124.0 ^{b)}
C(4)–C(m)	1.501(6)	C(2)–N–C(6)	115.8 ^{b)}
C(2)–H	1.101(4)	C(3)–C(2)–H	121.2(16)
C(3)–H	1.099(4)	C(4)–C(3)–H	122.2(16)
C(m)–H	1.109(4)	C(4)–C(m)–H	110.9 ^{c)}

It was assumed that the pyridine ring with the methyl carbon is planar and the methyl group has C_{3v} symmetry and no tilt. The methyl rotation was treated as a large-amplitude motion. The differences in the C–C distances of the ring, in the C–H distances, in the C–C–C and C–C–H bond angles of the ring were assumed at the values from RHF/6-311G** calculations. The nozzle temperature was 75 °C.

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

^{b)} Dependent parameter.

^{c)} Assumed at the value from RHF/6-311G** calculations.



Inoue, K., Kuze, N., Tanabe, M., Takeuchi, H., Egawa, T., Konaka, S.: J. Mol. Struct. **413-414** (1997) 81.