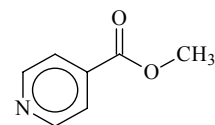


803 **C₇H₇NO₂**ED, *ab initio*
calculations**Methyl isonicotinate**4-Pyridinecarboxylic acid methyl ester
Isonicotinic acid methyl ester**C_s** assumed

r_g	Å ^{a)}	θ_α	deg ^{a)}
N–C	1.343(5)	C–N–C	117.6(9)
C–C (ring)	1.401(3)	N–C–C	123.6 ^{b)}
C(4)–C(7)	1.499(9)	C(2)–C(3)–C(4)	118.2 ^{b)}
C(7)=O(8)	1.205(5)	C(3)–C(4)–C(5)	118.7(9)
C(7)–O(9) ^{c)}	1.331(8)	C(3)–C(4)–C(7)	118.6(12)
O(9)–C(10) ^{c)}	1.430(8)	C(4)–C(7)=O(8)	121.4(12)
C–H (ring) ^{d)}	1.101(10)	C(4)–C(7)–O(9)	114.2(10)
C–H (methyl) ^{d)}	1.107(10)	C(7)–O(9)–C(10)	115.4(15)
		C(3)–C(2)–H ^{e)}	120.6 ^{f)}
		O(9)–C(10)–H	108.8 ^{f)}

Local C_{2v} symmetry for the pyridine ring and local C_{3v} symmetry and the staggered conformation for the methyl group were assumed.

The temperature of the nozzle was 367 K.

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

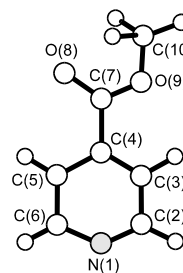
^{b)} Dependent parameter.

^{c)} Difference between O(9)–C(10) and C(7)–O(9) distances was assumed at the value from RHF/6-31G* calculations.

^{d)} Difference between the C–H distance in the ring and that in the methyl group was assumed at the value from RHF/6-31G* calculations.

^{e)} The C(3)–C(2)–H and C(4)–C(3)–H angles were assumed to be equal.

^{f)} Assumed at the value from RHF/6-31G* calculations.



Kiyono, H., Kuze, N., Fujiwara, H., Takeuchi, H., Egawa, T., Konaka, S.: J. Mol. Struct. **376** (1996) 145.