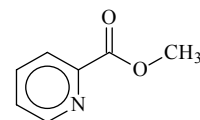


801 **C₇H₇NO₂**ED, *ab initio*
calculations**2-Pyridinecarboxylic acid methyl ester**Picolinic acid methyl ester
Methyl picolinate**C_s (*anti*)****C_s (*syn*)**

r_g	$\text{\AA}^a)$		θ_α	$\text{deg}^a)$	
	<i>anti</i>	<i>syn</i>		<i>anti</i>	<i>syn</i>
N(1)–C(2)	1.346(7)	1.347(7)	C(2)–N(1)–C(6)	117.2(12)	117.5(12)
N(1)–C(6)	1.342(7)	1.339(7)	N(1)–C(2)–C(3)	124.0(12)	123.7(12)
C(2)–C(3)	1.399(4)	1.399(4)	N(1)–C(6)–C(5)	123.8(12)	123.8(12)
C(5)–C(6)	1.401(4)	1.402(4)	C(2)–C(3)–C(4) ^{b)}	117.3	117.3
C(3)–C(4)	1.397(4)	1.399(4)	C(6)–C(5)–C(4) ^{b)}	117.7	117.5
C(4)–C(5)	1.396(4)	1.394(4)	C(3)–C(4)–C(5) ^{b)}	120.0	120.2
C(2)–C(7)	1.497(11)	1.500(11)	N–C(2)–C(7)	115.1(10)	118.8(10)
C(7)=O(8)	1.209(7)	1.205(7)	C(2)–C(7)=O(8)	121.0(12)	123.8(12)
C(7)–O(9)	1.328(11)	1.342(11)	C(2)–C(7)–O(9)	115.1(12)	113.5(12)
O(9)–C(10)	1.431(11)	1.432(11)	C(7)–O(9)–C(10)	115.4 ^{c)}	115.2
C–H (ring)	1.093(13)	1.093(13)	N–C(6)–H	116.2 ^{d)}	116.3 ^{d)}
C(10)–H	1.099(13)	1.099(13)	C(2)–C(3)–H	119.8 ^{d)}	120.5 ^{d)}
			C(3)–C(4)–H	120.5 ^{d)}	120.4 ^{d)}
			C(4)–C(5)–H	121.4 ^{d)}	121.5 ^{d)}
			O–C–H	108.9 ^{e)}	109.0 ^{e)}
			$\tau^f)$	180.0 ^{d)}	0.0 ^{d)}

The molecule exists as a mixture of *anti* (77(23) mol%) and *syn* conformers. The pyridine ring and O=C–O–C fragment were assumed to be planar. Local C_{3v} symmetry was assumed for the methyl group. Differences between the corresponding parameters of *anti* and *syn* conformers and differences between the similar parameters in each conformer were assumed at the values derived from RHF/6-31G* calculations. The energy difference $\Delta E(\textit{syn} - \textit{anti})$ was estimated to be 1.65 kcal mol^{−1} by RHF/6-31G* calculations. The nozzle temperature was 343 K.

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

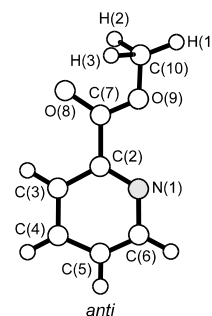
^{b)} Dependent parameter.

^{c)} Assumed at the value for methyl isonicotinate.

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

^{e)} Assumed at the average of the values from RHF/6-31G* calculations.

^{f)} Torsional angle N(1)–C(2)–C(7)=O(8).



Kiyono, H., Tatsunami, R., Kurai, T., Takeuchi, H., Egawa, T., Konaka, S.: J. Phys. Chem. A **102** (1998) 1405.