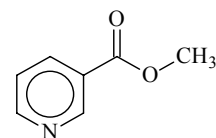


802 $C_7H_7NO_2$ ED, *ab initio*
calculations

3-Pyridinecarboxylic acid methyl ester

Nicotinic acid methyl ester
Methyl nicotinate 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)	1.336(7)	1.334(7)	C(2)–N(1)–C(6)	119.0(14)	119.0(14)
N(1)–C(6)	1.337(7)	1.338(7)	N(1)–C(2)–C(3)	122.5(11)	122.7(11)
C(2)–C(3)	1.405(3)	1.406(3)	N(1)–C(6)–C(5)	123.0(11)	123.0(11)
C(5)–C(6)	1.401(3)	1.400(3)	C(2)–C(3)–C(4) ^{b)}	118.5	118.4
C(3)–C(4)	1.405(3)	1.404(3)	C(6)–C(5)–C(4) ^{b)}	118.6	118.6
C(4)–C(5)	1.396(3)	1.398(3)	C(3)–C(4)–C(5) ^{b)}	118.5	118.5
C(3)–C(7)	1.480(12)	1.480(12)	C(2)–C(3)–C(7)	118.3(12)	123.8(12)
C(7)=O(8)	1.199(7)	1.198(7)	C(3)–C(7)=O(8)	121.5(12)	121.9(12)
C(7)–O(9)	1.332(11)	1.334(11)	C(3)–C(7)–O(9)	115.6(10)	115.3(10)
O(9)–C(10)	1.428(11)	1.428(11)	C(7)–O(9)–C(10)	115.4 ^{c)}	115.3
C–H (ring)	1.092(12)	1.092(12)	C(3)–C(2)–H	120.3 ^{d)}	119.5 ^{d)}
C(10)–H	1.098(12)	1.098(12)	C(3)–C(4)–H	119.6 ^{d)}	120.4 ^{d)}
			C(4)–C(5)–H	121.5 ^{d)}	121.3 ^{d)}
			C(5)–C(6)–H	120.2 ^{d)}	120.2 ^{d)}
			O–C–H	108.8 ^{e)}	108.9 ^{e)}
			$\tau^f)$	180.0 ^{d)}	0.0 ^{d)}

The molecule exists as a mixture of *anti* (66(34) 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 $\Delta E(\text{syn} - \text{anti})$ was estimated to be 0.29 kcal mol^{−1} by RHF/6-31G* calculations. The nozzle temperature was 341 K.

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

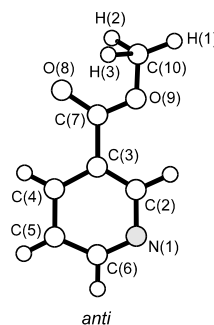
^{b)} Dependent parameter.

^{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 C(2)–C(3)–C(7)=O(8).



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