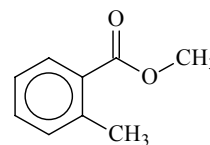


872  $C_9H_{10}O_2$   
ED, *ab initio*  
calculations

**2-Methylbenzoic acid methyl ester**  
Methyl 2-methylbenzoate

essentially  $C_s$  (*sp*)  
essentially  $C_s$  (*ap*)



$r_a$	$\text{\AA}^a$		$\theta_a$	$\text{deg}^a$	
	<i>sp</i>	<i>ap</i>		<i>sp</i>	<i>ap</i>
C(1)–C(2)	1.412(3)	1.413(3)	C(2)–C(1)–C(6)	120.2(10)	120.2(5)
C(1)–C(8)	1.482(7)	1.487(5)	C(1)–C(2)–C(3)	115.7(15)	115.4(14)
C(1)–C(6)	1.404(3)	1.403(3)	C(2)–C(3)–C(4)	124.5(12)	124.8(14)
C(5)–C(6)	1.391(3)	1.390(3)	C(1)–C(2)–C(7)	123.1(16)	124.3(12)
C(4)–C(5)	1.394(3)	1.394(3)	C(2)–C(1)–C(8)	122.8(10)	127.9(8)
C(3)–C(4)	1.393(3)	1.393(3)	C(1)–C(8)=O(9)	126.2(17)	127.6(19)
C(2)–C(3)	1.401(3)	1.402(3)	C(1)–C(8)–O(10)	111.8(21)	110.2(21)
C(2)–C(7)	1.497(7)	1.499(5)	C(8)–O(10)–C(11)	118.9(21)	119.0(21)
C(8)=O(9)	1.222(3)	1.222(3)	H–C–H (mean)	110.7(7)	110.7(7)
C(8)–O(10)	1.358(7)	1.354(7)	$\tau_1^b$ $^c$	29.1(21)	150.9(21)
C(11)–O(10)	1.439(7)	1.440(7)	$\tau_2^c$ $^d$	–175.5(71)	–175.5(71)
C–H (mean)	1.099(3)	1.099(3)	$\tau_3^c$ $^e$	41.3(85)	41.3(85)
			$\tau_4^c$ $^f$	41.3(85)	41.3(85)

The molecule was found to exist as a mixture of two conformers with different torsional angles around the C(1)–C(8) bond, *sp* (73(14)%) and *ap* (27(14)%). Local  $C_{3v}$  symmetry was assumed for the C–CH<sub>3</sub> and O–CH<sub>3</sub> groups. Differences between the corresponding parameters of the two conformers and differences between the bond lengths of the heavy-atom skeleton were assumed at the values from MP2/6-311++G\*\* calculations. The energy difference between the *ap* and *sp* conformers was calculated to be 3.7 kJ mol<sup>–1</sup> by MP2/6-311++G\*\* method. According to *ab initio* calculations, these conformers have planar skeletons. The nonplanar structure derived from ED, a thermal average over torsional vibrations, can be made compatible with the planar equilibrium structure derived from *ab initio* calculations. The nozzle temperature was *ca.* 320 K.

<sup>a</sup>) 1.4 times the estimated standard errors including a systematic error.

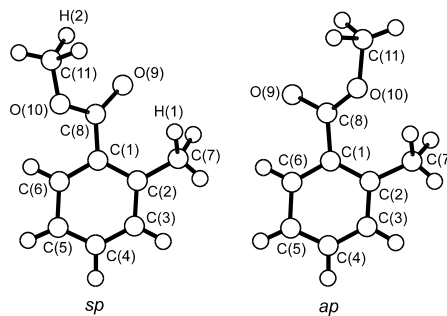
<sup>b</sup>) Torsional angle C(2)–C(1)–C(8)–O(9).

<sup>c</sup>) Zero degree for the eclipsed position, positive value for the clockwise rotation.

<sup>d</sup>) Torsional angle C(1)–C(8)–O(10)–C(11).

<sup>e</sup>) Torsional angle C(1)–C(2)–C(7)–H(1).

<sup>f</sup>) Torsional angle C(8)–O(10)–C(11)–H(2).



Hnyk, D., Borisenko, K.B., Samdal, S., Exner, O.: Eur. J. Org. Chem. (2000) 2063.