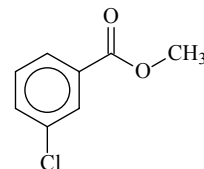


830 **C₈H₇ClO₂**ED, *ab initio*
calculations**3-Chlorobenzoic acid methyl ester**Methyl 3-chlorobenzoate
Methyl *m*-chlorobenzoateC_s assumed (*s-anti*)C_s assumed (*s-syn*)

| r_g | Å ^{a)} | θ_α | deg ^{a)} |
|-------------|-----------------|------------------|---------------------|
| C(2)–H | 1.101(10) | C(6)–C(1)–C(2) | 120.7(2) |
| C(4)–H | 1.102(10) | C(1)–C(2)–C(3) | 118.6(2) |
| C(5)–H | 1.103(10) | C(1)–C(6)–C(5) | 119.4(2) |
| C(6)–H | 1.102(10) | C(2)–C(3)–C(4) | 121.6 ^{b)} |
| C(11)–H(1) | 1.105(10) | C(3)–C(4)–C(5) | 118.8 ^{b)} |
| C(11)–H(2) | 1.108(10) | C(4)–C(5)–C(6) | 120.8 ^{b)} |
| C(1)–C(2) | 1.398(2) | C(2)–C(1)–C(8) | 117.3(14) |
| C(2)–C(3) | 1.392(2) | C(1)–C(8)=O(9) | 122.2(14) |
| C(3)–C(4) | 1.395(2) | C(1)–C(8)–O(10) | 116.4(12) |
| C(4)–C(5) | 1.395(2) | C(8)–O(10)–C(11) | 114.9(19) |
| C(5)–C(6) | 1.392(2) | C(2)–C(3)–Cl(7) | 120.8(17) |
| C(6)–C(1) | 1.398(2) | C(1)–C(2)–H | 120.6 ^{c)} |
| C(1)–C(8) | 1.480(13) | C(1)–C(6)–H | 118.9 ^{c)} |
| C(8)=O(9) | 1.209(6) | C(6)–C(5)–H | 120.0 ^{c)} |
| C(8)–O(10) | 1.352(8) | C(5)–C(4)–H | 121.0 ^{c)} |
| O(10)–C(11) | 1.438(8) | O(10)–C(11)–H(1) | 105.1 ^{c)} |
| O(10)–C(11) | 1.438(8) | O(10)–C(11)–H(2) | 110.3 ^{c)} |
| C(3)–Cl(7) | 1.741(4) | | |

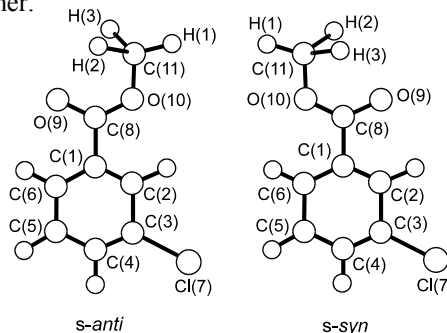


The molecule exists as a mixture of *s-anti* (70(23)%) and *s-syn* (30%) conformers. The skeleton of the O=C–O–CH₃ group was assumed to be planar. The differences between the corresponding parameters of the conformers and the differences between the similar parameters of each conformer were assumed at the values from MP2/6-31G** calculations. The parameters are listed for the *s-anti* conformer. The nozzle temperature was 370 K.

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

^{b)} Dependent parameter.

^{c)} Assumed at the values from MP2/6-31G** calculations.



Takashima, H., Endo, K., Ito, M., Takeuchi, H., Egawa, T., Konaka, S.: J. Mol. Struct. **478** (1999) 13.