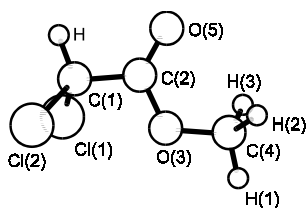


**1145**     **C<sub>3</sub>H<sub>4</sub>Cl<sub>2</sub>O<sub>2</sub>**  
ED, *ab initio* calculations  
(HF/6-31G\*)

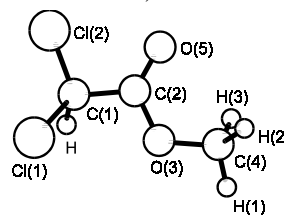
**Methyl dichloroacetate**

**C<sub>s</sub> (*syn*)**  
**C<sub>1</sub> (*gauche*)**  
Cl<sub>2</sub>HC–C(O)–O–CH<sub>3</sub>

<i>r<sub>g</sub></i>			<i>θ<sub>α</sub></i>		
Å <sup>a)</sup>			deg <sup>a)</sup>		
	<i>syn</i>	<i>gauche</i>		<i>syn</i>	<i>gauche</i>
C–H	1.108(13)	1.110(13)	O(3)–C(2)=O(5)	125.4(6)	125.2(15)
C(2)=O(5)	1.213(4)	1.208(4)	C(1)–C(2)=O(5)	122.0(11)	126.1(11)
C–C	1.528(7)	1.532(7)	C(2)–O(3)–C(4)	117.7(16)	117.5(16)
C(2)–O(3)	1.328(6)	1.336(6)	O–C–H	103.8(30)	103.9(30)
O(3)–C(4)	1.437(6)	1.438(6)	C–C–H	107.8 <sup>b)</sup>	109.8 <sup>b)</sup>
C–Cl	1.767(3)	1.774(3)	C–C–Cl(1)	109.9(6)	107.4(6)
			C–C–Cl(2)	109.9(6)	110.9(6)
			Cl–C–Cl	111.7(4)	111.6(4)
			φ <sub>1</sub> <sup>c)</sup>	0.0	152(5)
			φ <sub>2</sub> <sup>d)</sup>	0.0 <sup>b)</sup>	1.0 <sup>b)</sup>
			φ <sub>3</sub> <sup>e)</sup>	180 <sup>b)</sup>	179 <sup>b)</sup>



*syn*



*gauche*

Two conformers were identified, 53(13)% of a *syn* form and 47(13)% of a *gauche* form. The differences between corresponding bond distances and valence angles were fixed at the *ab initio* values. Local C<sub>3v</sub> symmetry was assumed for the methyl group. The nozzle was at 22...23 °C.

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

<sup>b)</sup> Fixed in the final refinement at the *ab initio* value.

<sup>c)</sup> Dihedral angle H–C(1)–C(2)–O(5), φ<sub>1</sub> = 0° for the *syn* position.

<sup>d)</sup> Dihedral angle C(4)–O(3)–C(2)–O(5), φ<sub>2</sub> = 0° for the *syn* position.

<sup>e)</sup> Dihedral angle H(1)–C(4)–O(3)–C(2)), φ<sub>3</sub> = 0° for the *syn* position.

Litvinov, O.A., Zuev, M.B., Naumov, V.A., Volden, H.V., Hagen, K.: J. Phys. Chem. **97** (1993) 10674.