

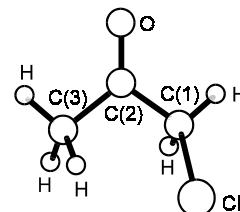
1196  
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**C<sub>3</sub>H<sub>5</sub>ClO**

**Chloroacetone**  
1-Chloro-2-propanone

**C<sub>1</sub> (*gauche*)**  
**C<sub>s</sub> (*syn*)** (except H atoms  
in CH<sub>3</sub> group)  
H<sub>3</sub>C–C(O)–CClH<sub>2</sub>

$r_g$	Å <sup>a)</sup>	$\theta_\alpha$	deg <sup>a)</sup>
C–H	1.109(7)	C(1)–C(2)=O	121.5(16)
C=O	1.216(3)	C–C–C	119.5(9)
C(1)–C(2)	1.537(18)	C–C–Cl	113.7(9)
C(2)–C(3)	1.507(16)	C(2)–C(3)–H	110.0 <sup>b)</sup>
C–Cl	1.787(3)	C(2)–C(1)–H	107(3)
		H–C(1)–H	109.0 <sup>b)</sup>
		$\tau_1$ ( <i>gauche</i> ) <sup>c)</sup>	138(7)
		$\tau_2$ <sup>d)</sup>	28(14)



The majority of the molecules have a *gauche* conformation (see figure); the amount of the *syn* conformation is 5(8)%. Only a small potential hump of 0.2(2) kcal mol<sup>−1</sup> separates the two equivalent *gauche* forms. C<sub>3v</sub> symmetry for the CH<sub>3</sub> group was assumed. The nozzle temperature was 322 K.

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

<sup>b)</sup> Assumed.

<sup>c)</sup> Cl–C–C=O torsion angle;  $\tau = 0^\circ$  for the *syn* conformer.

<sup>d)</sup> H–C(3)–C(2)=O torsion angle.

Shen, Q., Hagen, K.: J. Phys. Chem. **95** (1991) 7655.