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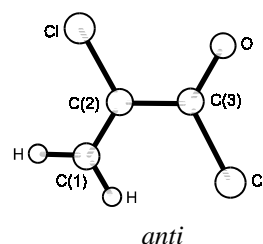
C₃H₂Cl₂O

2-Chloropropenoyl chloride

C_s

H₂C=CCl-C(O)Cl

r_g	Å ^{a)}	θ_α	deg ^{a)}
C(3)=O	1.189(2)	C-C=O	125.5(6)
C=C	1.342(3)	C=C-C	122.0(6)
C-C	1.496(3)	C(3)-C(2)-Cl	118.3(4)
C-Cl	1.753(2)	C(2)-C(3)-Cl	113.4(3)
$\Delta(C-Cl)$ ^{b)}	0.041(6)	$\Delta[C(2)-C(3)-Cl]$ ^{c)}	3.0 ^{d)}
C(3)-Cl	1.774(4)		
C(2)-Cl	1.733(4)		
C-H	1.115 ^{d)}		



Two conformers were identified, a more stable *anti* form (77.5(98)% at 303 K) and a less stable planar (or nearly planar) *syn* form. $\Delta E^\circ = E^\circ(\text{syn}) - E^\circ(\text{anti}) = 3.8$ ($\sigma = 2.2$) kJ mol⁻¹ and $\Delta S^\circ(\text{syn}) - S^\circ(\text{anti}) = 2.7$ ($\sigma = 5.6$) J mol⁻¹ K⁻¹. Different nozzle temperatures: 303, 373, 475 K. The parameters for a model comprising weighted averages of the results from the three temperatures are listed, since there was no systematic variation with temperature observed in these parameters.

^{a)} Twice the estimated standard errors.

^{b)} [C(3)-Cl] - [C(2)-Cl].

^{c)} [C(2)-C(3)-Cl(*syn*)] - [C(2)-C(3)-Cl(*anti*)].

^{d)} Assumed.

Hagen, K., Hedberg, K.: J. Am. Chem. Soc. **111** (1989) 6905.