

1089
ED, MW

C₃H₃ClO

Propenoyl chloride
Acryloyl chloride

C_s (*anti*)
C_s (*syn*)
H₂C=CH-C(O)Cl

r_a	Å ^{a)}	θ_α	deg ^{a)}
C=O	1.192(2)	C-C=O	125.2(2)
C=C	1.339(2)	C-C-Cl (<i>anti</i>)	116.3(8)
C-C	1.484(4)	C-C-Cl (<i>syn</i>)	111.8(15)
C-Cl (<i>anti</i>)	1.804(3)	C-C=C	123.4(7)
C-Cl (<i>syn</i>)	1.772(4)		
C-H	1.100(6)		

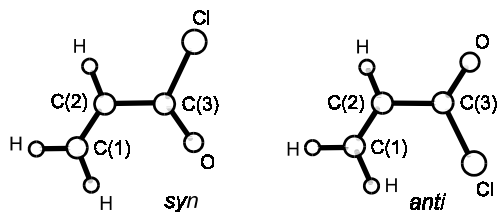
Two conformers were identified, a more stable planar *anti* form (60.5(66)% at 20 °C) and a less stable planar (or nearly planar) *syn* form.

$$E^\circ(\text{syn}) - E^\circ(\text{anti}) = 0.25(18) \text{ kcal mol}^{-1},$$

$$S^\circ(\text{syn}) - S^\circ(\text{anti}) = -0.15(5) \text{ cal mol}^{-1} \text{ K}^{-1}.$$

$V(\phi) = \frac{1}{2} \sum V_i (1 - \cos i\phi)$, $V_1 = 0.064$, $V_2 = 3.4$, $V_3 = 0.16$, all in kcal mol⁻¹ with uncertainties of about 0.2 kcal mol⁻¹.

Different nozzle temperatures: 20, 102, 207, 370 °C. The average parameters from four temperatures are listed.



^{a)} Twice the estimated standard errors.

Hagen, K., Hedberg, K.: J. Am. Chem. Soc. **106** (1984) 6150.

See also: (MW) Kewley, R., Hemphill, D.C., Curl, R.F.: J. Mol. Spectrosc. **44** (1972) 443.