

1582
MW

C₄H₅ClO

2-Methyl-2-propenoyl chloride
Methacryloyl chloride

C_s (*anti*)
H2C=C(CH3)-C(O)Cl

r_0	Å	θ_0	deg
C(1)=C(2)	1.342 ^{a)}	C(1)=C(2)-C(3)	122.7 ^{a)}
C(2)-C(4)	1.509 ^{a)}	C(1)=C(2)-C(4)	123.9 ^{a)}
C(2)-C(3)	1.492(7)	Cl-C(3)-C(2)	116.1(11)
C(3)-Cl	1.792(8)	O=C(3)-C(2)	123.9(15)
C(3)=O	1.191 ^{a)}	H(1)-C(1)=C(2)	122.9 ^{a)}
C(1)-H(1)	1.081 ^{a)}	H(2)-C(1)=C(2)	120.4 ^{a)}
C(1)-H(2)	1.085 ^{a)}	H(3)-C(4)-C(2)	110.3 ^{a)}
C(4)-H(3)	1.091 ^{a)}	H(4,5)-C(4)-C(2)	110.9 ^{a)}
C(4)-H(4,5)	1.092 ^{a)}	H(4)-C(4)-H(5)	107.2 ^{a)}

^{a)} Assumed.

Durig, J.R., Brletic, P.A., Li, Y.S., Wang, A.-Y., Little, T.S.: J. Mol. Struct. **223** (1990) 291.

ED

r_a	Å ^{a)}	θ_a	deg ^{a)}
C-H (mean)	1.100(7)	C-C=O	125.8(4)
$\Delta(\text{C-H})$ ^{b)}	0.01 ^{c)}	C-C-Cl	114.8(3)
C=O	1.189(3)	C-C-C	115.3(3)
C-C ^{d)}	1.497(2)	C-C=C	124.2(6)
$\Delta(\text{C-C})$ ^{e)}	0.02 ^{c)}	C=C-H	120.0 ^{c)}
C=C	1.336(3)	C-C-H	110.5 ^{c)}
C-Cl	1.792(3)		

The molecule exists as a mixture of two conformers, a more stable *anti* form, (*anti* and *syn* referring to the double bonds). Both forms are planar or near planar except for the CH₃ hydrogen atoms. Mole fraction of the *anti* form: 0.89(9) and 0.82(17) at 303 and 573 K, respectively.

$\Delta E^\circ = E^\circ(\text{syn}) - E^\circ(\text{anti}) = 3.3(39) \text{ kJ mol}^{-1}$ and

$\Delta S^\circ = S^\circ(\text{syn}) - S^\circ(\text{anti}) = -6.6(46) \text{ J mol}^{-1} \text{K}^{-1}$.

The nozzle temperatures were 303 and 573 K.

The parameters for 303 K are listed.

^{a)} Twice the estimated standard errors including a systematic error.

^{b)} $\Delta(\text{C-H}) = [\text{C}(4)\text{-H}] - [\text{C}(1)\text{-H}]$.

^{c)} Assumed.

^{d)} $(\text{C-C}) = 0.5[(\text{C}(2)\text{-C}(3)) + (\text{C}(2)\text{-C}(4))]$.

^{e)} $\Delta(\text{C-C}) = [\text{C}(2)\text{-C}(4)] - [\text{C}(2)\text{-C}(3)]$.

Postmyr, L., Hagen, K., Shen, Q.: J. Mol. Struct. **244** (1991) 17.

essentially C_s (*anti*)
essentially C_s (*syn*)

