

1581  
ED

**C<sub>4</sub>H<sub>5</sub>ClO**

**(E)-2-Butenoyl chloride**  
Crotonyl chloride

**C<sub>s</sub> (*anti*)**  
essentially C<sub>s</sub> (*syn*)  
H<sub>3</sub>C–CH=CH–C(O)Cl

$r_a$	Å <sup>a)</sup>	$\theta_\alpha$	deg <sup>a)</sup>
C–H	1.097(13)	C(2)–C(1)=O	125.8(7)
C(1)=O	1.199(4)	C(2)–C(1)–Cl	114.4(6)
C(2)=C(3)	1.349(7)	C(1)–C(2)=C(3)	126.8(14)
C(1)–C(2)	1.473(9)	C(2)=C(3)–C(4)	123.0(16)
C(3)–C(4)	1.517(8)	C(2)=C(3)–H	122.0 <sup>b)</sup>
C(1)–Cl	1.800(6)	C(3)–C(4)–H	112.1(40)
		$\tau$ ( <i>syn</i> ) <sup>c)</sup>	160.8(158)
		$\phi$ <sup>d)</sup>	0.0 <sup>b)</sup>
		$\delta$ ( <i>anti</i> ) <sup>e)</sup>	19.6(130)

The molecule exists as a mixture of two conformers with the C(3)=C(2) and C(1)=O double bonds *anti* (53(11)%) or *syn* to each other.

The nozzle temperature was 343 K.

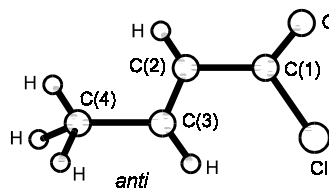
<sup>a)</sup> Twice the estimated standard errors including a systematic error.

<sup>b)</sup> Assumed.

<sup>c)</sup> O=C–C=C torsion angle of the *syn* conformer;  $\tau = 0^\circ$  when C=O and C=C bonds are *anti* to each other.

<sup>d)</sup> C(2)=C(3)–C(4)–H torsion angle;  $\phi = 0^\circ$  when one of the C(4)–H bonds is eclipsed with respect to the C(3)=C(2) bond.

<sup>e)</sup> The root-mean-square amplitude of the torsional angle O=C–C=C for the *anti* conformer.



Nordtømme, T., Hagen, K.: J. Mol. Struct. **128** (1985) 127.