

1634  
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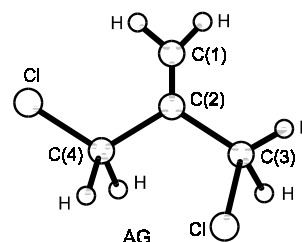
$C_4H_6Cl_2$

3-Chloro-2-chloromethyl-1-propene

$C_2$  (GG)  
 $C_1$  (AG)  
 $H_2C=C(CH_2Cl)_2$

$r_a$	$\text{\AA}^a$
C–H	1.088(12)
C=C	1.331(10)
C–C	1.502(6)
C–Cl	1.799(4)

$\theta_a$	deg <sup>a)</sup>
C–C–C	121(1)
C–C–Cl	111.5(6)
H–C–H	109.5 <sup>b)</sup>
C=C–H	120.0 <sup>b)</sup>
$\varphi$ <sup>c)</sup>	130.0 <sup>b)</sup>
$\tau_{2-3}$ (GG) <sup>d)</sup>	115(3)
$\tau_{2-3}$ (AG) <sup>d)</sup>	120.0 <sup>b)</sup>
$\tau_{2-4}$ (AG) <sup>d)</sup>	7(21)



The molecule exists as a mixture of GG (66(19)%) and AG (34(19)%) conformers.  
The nozzle temperature was 90 °C.

<sup>a)</sup> Uncertainties unidentified, possibly three times the estimated standard errors.

<sup>b)</sup> Assumed.

<sup>c)</sup> Angle between the C(2)–C(3) bond and the HC(3)H plane.

<sup>d)</sup> C(1)=C(2)–C(3,4)–Cl torsional angles,  $\tau = 0^\circ$  when C–Cl bond is eclipsed with respect to the C(1)=C(2) bond;  $\tau_{2-3} = \tau_{2-4}$  for the GG conformer.

Shen, Q.: J. Mol. Struct. **53** (1979) 61.