

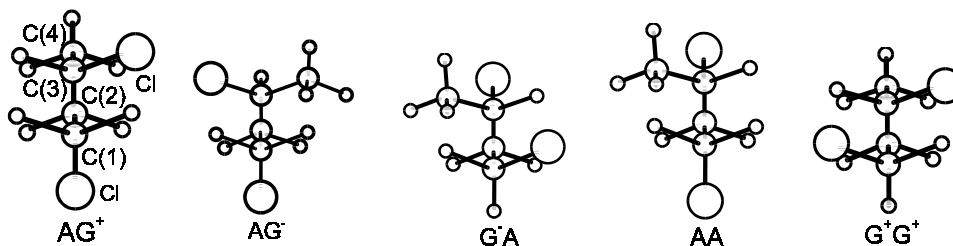
**1723 C<sub>4</sub>H<sub>8</sub>Cl<sub>2</sub>**

 ED, *ab initio* calculations  
(HF/6-31G\*)

**1,3-Dichlorobutane**

 C<sub>1</sub> (all conformers)  
ClH<sub>2</sub>C–CH<sub>2</sub>–CHCl–CH<sub>3</sub>

$r_g$	$\text{\AA}^a$	$\theta_\alpha$	deg <sup>a)</sup>
C(1)–C(2)	1.524(3)	C(1)–C(2)–C(3)	114.5(7)
C(2)–C(3)	1.527(3)	C(2)–C(3)–C(4)	111.0(7)
C(3)–C(4)	1.530(3)	C(2)–C(1)–Cl	112.1(6)
C(1)–Cl	1.799(3)	C(2)–C(3)–Cl	109.9(6)
C(3)–Cl	1.810(3)	C–C–H (average)	111.9(20)
C–H (average)	1.083(11)		



This molecule may in principle exist as a mixture of nine different conformers; five of them ( $G^+G^+$  (54(20)%)  $AG^+$  (14(25)%),  $G^-A$  (17(24)%),  $AG^-$  (4(15)%), and  $AA$  (10(22)%) were included in the analysis. The first and second symbols refer to torsion about the C(1)–C(2) and C(2)–C(3) bonds, respectively. The symbols refer to *anti* (A) with a torsion angle of about 180° and *gauche* ( $G^+$  and  $G^-$ ) with torsion angles of about +60° and –60°, respectively. Only the average values for C–C, C–Cl, C–H, C–C–C, C–C–Cl and C–C–H were refined in the least-squares analysis; the differences between the values for these parameters in the same conformer and those between different conformers were fixed at the corresponding *ab initio* values.

Parameters are given for the predominant  $G^+G^+$  conformer.

The nozzle temperature was 28 °C.

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

Aarset, K., Hagen, K., Stølevik, R.: J. Phys. Chem. **99** (1995) 11089.