

| $r_g [\text{\AA}]^a)$ | AA                  | AG                  | GA                  | GG                  |
|-----------------------|---------------------|---------------------|---------------------|---------------------|
| C–H <sup>b)</sup>     | 1.109 <sup>c)</sup> | 1.109 <sup>c)</sup> | 1.109 <sup>c)</sup> | 1.109 <sup>c)</sup> |
| C(1)–C(2)             | 1.507(7)            | 1.509(7)            | 1.509(7)            | 1.512(7)            |
| C(2)–C(3)             | 1.506(7)            | 1.508(7)            | 1.510(7)            | 1.512(7)            |
| C–Br                  | 1.954(14)           | 1.959(14)           | 1.953(14)           | 1.959(14)           |
| C–Cl                  | 1.811(10)           | 1.810(10)           | 1.806(10)           | 1.814(10)           |

| $\theta_\alpha [\text{deg}]^a)$ | AA                  | AG                  | GA                  | GG                  |
|---------------------------------|---------------------|---------------------|---------------------|---------------------|
| C–C–H <sup>b)</sup>             | 109.0 <sup>c)</sup> | 109.0 <sup>c)</sup> | 109.0 <sup>c)</sup> | 109.0 <sup>c)</sup> |
| H–C–H <sup>b)</sup>             | 105.0 <sup>c)</sup> | 105.0 <sup>c)</sup> | 105.0 <sup>c)</sup> | 105.0 <sup>c)</sup> |
| C–C–C                           | 115.1(35)           | 115.8(35)           | 116.0(33)           | 116.2(33)           |
| C–C–Br                          | 111.6(9)            | 111.7(9)            | 112.7(9)            | 113.0(9)            |
| C–C–Cl                          | 111.9(8)            | 112.7(8)            | 112.0(8)            | 112.9(8)            |
| $\varphi_1^d)$ <sup>e)</sup>    | 10.0 <sup>c)</sup>  | 29.9(250)           | 119.3(439)          | 119.3(100)          |
| $\varphi_2^e)$ <sup>f)</sup>    | –5.0 <sup>c)</sup>  | 215.4(289)          | –15.3(153)          | 246.3(89)           |

The molecule exists as a conformational mixture of the AA, AG, GA and GG conformers in the estimated ratio 1:3:1:5, respectively. The symbols refer to *anti* (A) and *gauche* (G) dihedral angles at the C(1)–C(2) and C(2)–C(3) bonds. Differences between (and conformational variations within) the C(1)–C(2) and C(2)–C(3) bond lengths and the conformational variations within the C–C–Br, C–C–Cl and C–C–C bond angles and the C–Br and C–Cl bond lengths, were fixed at the values derived from MM calculations. The nozzle temperature was 23–27 °C.

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

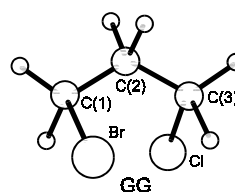
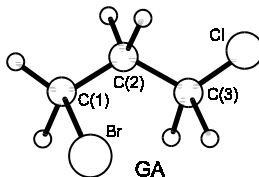
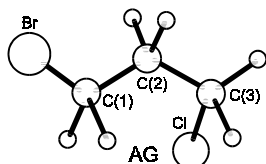
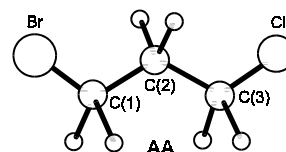
<sup>b)</sup> Assumed conformationally equal.

<sup>c)</sup> Not refined.

<sup>d)</sup> Torsion angle Br–C(1)–C(2)–C(3).

<sup>e)</sup> 0° for *anti* position.

<sup>f)</sup> Torsion angle Cl–C(3)–C(2)–C(1).



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