

1000
ED

$C_3Cl_2F_6$

1,3-Dichloro-1,1,2,2,3,3-hexafluoropropane

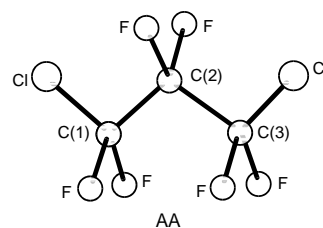
C_{2v} (AA)

C_2 (GG)

C_1 (AG)

$F_2ClC-CF_2-CF_2Cl$

| r_g | \AA^a | θ^b | deg^a |
|-------|----------------|---------------|---------------------|
| C–F | 1.337(2) | C–C–C | 114.3(10) |
| C–C | 1.560(3) | C–C–Cl | 109.9(4) |
| C–Cl | 1.755(3) | C–C–F | 108.9(4) |
| | | F–C(2)–F | 106.6(10) |
| | | F–C(1,3)–F | 120.0 ^{c)} |
| | | $\tau_1^d)^e$ | 112.8(24) |
| | | $\tau_2^e)^f$ | 3.6(12) |



The molecule exists as a mixture of AA (53(6)%), AG (39(8)%) and GG (less than 10%) conformers.

The nozzle temperature was 20 °C.

^{a)} Estimated standard errors including a systematic error.

^{b)} Unidentified, possibly θ_a .

^{c)} Assumed.

^{d)} Torsional angle Cl–C(1)–C(2)–C(3) of the AG conformer.

^{e)} $\tau = 0^\circ$ for *anti* position.

^{f)} Torsional angle Cl–C(3)–C(2)–C(1) of the AG conformer.

Fernholt, L., Seip, R., Stølevik, R.: Acta Chem. Scand. Ser. A **32** (1978) 225.