

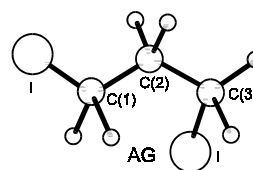
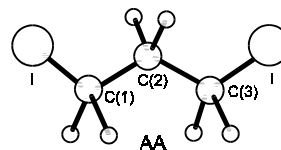
1254 $\text{C}_3\text{H}_6\text{I}_2$
ED, MM calculations

1,3-Diiodopropane

C_2 (AA, GG)
 C_1 (AG)
 $\text{IH}_2\text{C}-\text{CH}_2-\text{CH}_2\text{I}$

r_g [Å] ^{a)}	AA	AG	GG
C–H ^{b)}	1.139(47)	1.139(47)	1.139(47)
C–C	1.524(18)	1.522(18)	1.512(18)
C(1)–I	2.145(11)	2.153(11)	2.159(11)
C(3)–I	2.145(11)	2.158(11)	2.159(11)

θ_α [deg] ^{a)}	AA	AG	GG
C–C–H ^{b)}	109.0 ^{c)}	109.0 ^{c)}	109.0 ^{c)}
H–C–H ^{b)}	105.0 ^{c)}	105.0 ^{c)}	105.0 ^{c)}
C–C–C	111.0(49)	111.7(49)	112.6(49)
C(2)–C(1)–I	114.2(13)	114.4(13)	115.6(13)
C(2)–C(3)–I	114.2(13)	115.2(13)	115.6(13)
φ_1 ^{d)} ^{e)}	10.0 ^{c)}	–7.4(164)	114.9(61)
φ_2 ^{e)} ^{f)}	–10.0 ^{c)}	260.1(258)	–114.9(61)



The molecule exists as a conformational mixture of the AA (5.3(88)%), AG (39.5(211)%) and GG (55.2(237)%) conformers. 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–C–C and C–C–I bond angles and the C–I bond lengths were fixed at the values derived from MM calculations. The nozzle temperature was 37...39 °C.

^{a)} Twice the estimated standard errors including a systematic error.

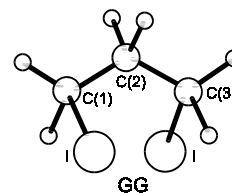
^{b)} Assumed conformationally equal.

^{c)} Not refined.

^{d)} Torsion angle I–C(1)–C(2)–C(3).

^{e)} 0° for *anti* position.

^{f)} Torsion angle I–C(3)–C(2)–C(1).



Postmyr, L.: J. Mol. Struct. **319** (1994) 211.