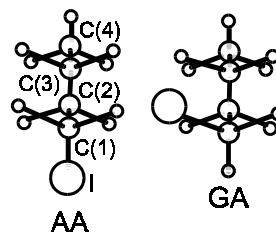


1787 **C₄H₉I**
ED, *ab initio* calculations
(HF/LANL1DZ)

1-Iodobutane
Butyl iodide

C₁ (GA, GG)
C_s (AA)
H₃C–CH₂–CH₂–CH₂I

<i>r_g</i>	Å ^a	<i>θ_α</i>	deg ^a
C(1)–C(2)	1.506(5)	C(1)–C(2)–C(3)	116.8(15)
C(2)–C(3)	1.518(5)	C(2)–C(3)–C(4)	115.3(15)
C(3)–C(4)	1.535(5)	C–C–I	110.2(14)
C–I	2.133(11)	C–C(1)–H	108.3(39)
C(1)–H	1.118(11)	C–C(2)–H	108.1(39)
C(2)–H	1.132(11)	C–C(3)–H	108.4(39)
C(3)–H	1.141(11)	C–C(4)–H	107.0(39)
C(4)–H	1.135(11)	I–C(1)–C(2)–C(3)	77(9)
		C(1)–C(2)–C(3)–C(4)	176(10)



The compound exists as a mixture of AA (19(17)%), GA (17(31)%), and GG (64(31)%) conformers, where the first and the second symbols refer to torsions about the C(1)–C(2) and C(2)–C(3) bonds, respectively. The symbols refer to *anti* (A) with the torsion angle of about 180° and *gauche* (G) with torsion angle of about 60°. Differences between the same set of parameters, C–C, C–H, C–C–C and C–C–H in the same conformer and those between different conformers were all fixed at the *ab initio* values.

Parameters are given for the *gauche-anti* conformer.

The nozzle temperature was 23 °C.

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

Aarset, K., Hagen, K., Stølevik, R., Sæbø, P.C.: Struct. Chem. **6** (1995) 197.

