

1773 C₄H₉Br
ED, *ab initio* calculations
(HF/6-31G* (H,C),
HF/6-31G*/Binning (Br))

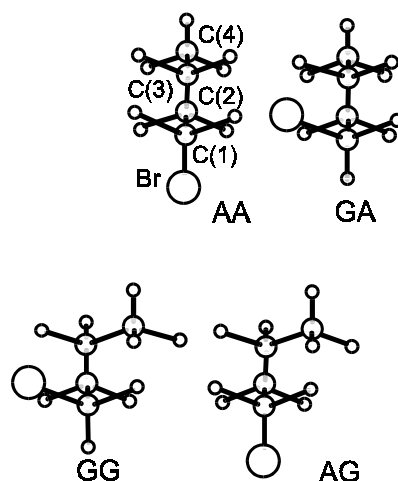
1-Bromobutane
Butyl bromide

C₁ (GA, GG, AG)
C_s (AA)
BrH₂C–CH₂–CH₂–CH₃

r_g	Å ^a	θ_α	deg ^a
C(1)–C(2)	1.513(4)	C(1)–C(2)–C(3)	115.3(11)
C(2)–C(3)	1.526(4)	C(2)–C(3)–C(4)	112.8(11)
C(3)–C(4)	1.540(4)	C–C–Br	112.1(14)
C–Br	1.959(8)	C–C(1)–H	113.4(43)
C(1)–H	1.104(8)	C–C(2)–H	108.7(43)
C(2)–H	1.118(9)	C–C(3)–H	109.3(43)
C(3)–H	1.134(9)	C–C(4)–H	112.6(43)
C(4)–H	1.110(9)	Br–C(1)–C(2)–C(3)	68(5)
		C(1)–C(2)–C(3)–C(4)	170(21)

The molecule exists as a mixture of AA (21(14)%), GA (33(32)%), AG (8(12)%) and GG (38(34)%) 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 that 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 18 °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.