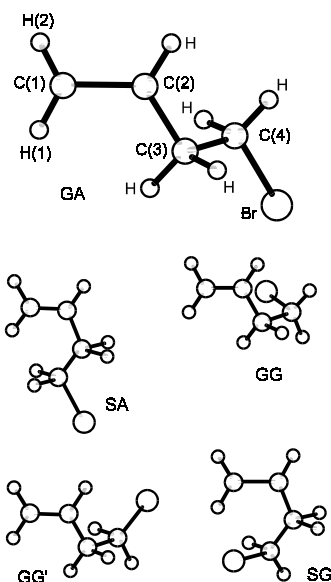


r_a	Å ^{a)}	θ_α	deg ^{a)}
C(1)=C(2)	1.339(10)	C(1)=C(2)-C(3)	122.9(32) ^{c)}
C(2)-C(3)	1.508(7)	C(2)-C(3)-C(4)	111.5(27) ^{c)}
C(3)-C(4)	1.528 ^{b)}	C(3)-C(4)-Br	111.2(7) ^{c)}
C(4)-Br	1.945(8)	C(2)=C(1)-H(1)	121.5 ^{d)}
C-H	1.092(11)	C(2)=C(1)-H(2)	121.1 ^{d)}
		C(1)=C(2)-H	119.0 ^{d)}
		C(2)-C(3)-H	110.4 ^{d)}
		C(4)-C(3)-H	110.3 ^{d)}
		C(3)-C(4)-H	111.7 ^{d)}
		Br-C(4)-H	106.3 ^{d)}
		C(1)=C(2)-C(3)-C(4)	120.0(36)
		C(2)-C(3)-C(4)-Br	180.0 ^{e)}

Molecular mechanics (MM) calculations showed that all the five distinct conformers (see figure) had energy differences of less than 7 kJ mol⁻¹. The most abundant form GA is found by the ED experiment to contribute 38(10)% to the conformational mixture, while the two forms with a planar arrangement of all the C atoms, SA and SG, comprise less than 15% together. The experimental data also show the presence of two forms having both the carbon skeleton and the Br atom in the *gauche* position, GG and GG'. Their total amount is ≈ 50%, but the separate amounts remain uncertain. The structure of the most abundant conformer, GA with a *gauche* carbon skeleton and an *anti* Br atom, is listed. The nozzle temperature was 23 °C.



- ^{a)} Twice the estimated standard errors including a systematic error.
^{b)} Assumed to be 0.02 Å longer than C(2)-C(3).
^{c)} Conformational differences were assumed to be those derived from molecular mechanics calculations for the other forms.
^{d)} Value from MM calculations.
^{e)} Assumed.

Schei, S.H.: J. Mol. Struct. **128** (1985) 151.