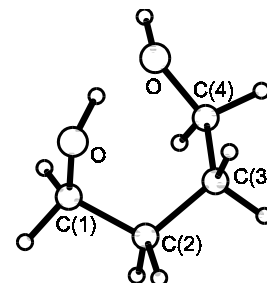


**1823**     **C<sub>4</sub>H<sub>10</sub>O<sub>2</sub>**  
ED, MM2 calculations

**1,4-Butanediol**

**C<sub>1</sub> (G<sup>+</sup>G<sup>-</sup>G<sup>-</sup>)**  
HO-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-OH

<i>r<sub>a</sub></i>	Å <sup>a)</sup>	<i>θ</i> <sup>c)</sup>	deg <sup>a)</sup>
C-O	1.426(2) <sup>b)</sup>	H-C-H	102.3(49) <sup>b)</sup>
C-C	1.528(2) <sup>b)</sup>	C-O-H	104.5 <sup>b)</sup> <sup>d)</sup>
O-H	1.014(35) <sup>b)</sup>	O-C-C	110.1(8) <sup>e)</sup>
C-H	1.106(12) <sup>b)</sup>	C-C-C	112.5(8) <sup>e)</sup>
		O-C-C	110.9(16) <sup>f)</sup>
		C-C-C	114.6(19) <sup>f)</sup>
		O-C(1)-C(2)-C(3)	67.0(54) <sup>g)</sup>
		C(1)-C(2)-C(3)-C(4)	-69.9(90) <sup>g)</sup>
		C(2)-C(3)-C(4)-O	-27.2(156) <sup>g)</sup>
		H-O-C(1)-C(2)	60.0 <sup>g)</sup>
		C(3)-C(4)-O-H	60.0 <sup>g)</sup>



G<sup>+</sup>G<sup>-</sup>G<sup>-</sup>

The molecule was expected to exist as a mixture of ten conformers. The relative population of the dominant conformer(s), G<sup>+</sup>G<sup>-</sup>G<sup>-</sup> (and/or G<sup>+</sup>G<sup>-</sup>G<sup>+</sup>), was estimated to be 40.2(43)% by an analysis of the experimental data measured at the nozzle temperature of 144...146 °C. Those of other conformers, estimated using molecular mechanics (MM2) calculations, were AAA (8.7%), AAG (18.4%), G<sup>+</sup>AG<sup>-</sup> (8.1%), G<sup>+</sup>AG<sup>+</sup> (5.3%), AGA (5.0%), AGG (5.9%), AG<sup>+</sup>G<sup>-</sup> (5.1%), and GGG (3.3%). The symbols refer to the *anti* (A) and *gauche* (G<sup>+</sup> or G<sup>-</sup>) dihedral angles at the C(1)-C(2), C(2)-C(3), and C(3)-C(4) bonds. It was impossible to distinguish two hydrogen-bonded conformers (G<sup>+</sup>G<sup>-</sup>G<sup>-</sup> and G<sup>+</sup>G<sup>-</sup>G<sup>+</sup>) by ED, but G<sup>+</sup>G<sup>-</sup>G<sup>-</sup> was suggested to be the dominant conformer, and the energy of the O-H...O-H internal hydrogen bonding was roughly estimated to be 10...11 kJ mol<sup>-1</sup>.

The structural data were also reported for measurement at 258...260 °C.

<sup>a)</sup> Twice the estimated standard errors.

<sup>b)</sup> Mean values for all conformers.

<sup>c)</sup> Unidentified, possibly  $\theta_{\alpha}$ .

<sup>d)</sup> Assumed.

<sup>e)</sup> Valence angles for the AAA conformer; differences between the corresponding angles for AAA and other conformers, except G<sup>+</sup>G<sup>-</sup>G<sup>+</sup> and G<sup>+</sup>G<sup>-</sup>G<sup>-</sup>, were assumed at the values from molecular mechanics calculations.

<sup>f)</sup> Valence angles for the hydrogen-bonded G<sup>+</sup>G<sup>-</sup>G<sup>-</sup> conformer.

<sup>g)</sup> Torsion angles for the G<sup>+</sup>G<sup>-</sup>G<sup>-</sup> conformer; the heavy atom torsion angles for other conformers were assumed at the MM2 values.

Trættemberg, M., Hedberg, K.: J. Am. Chem. Soc. **116** (1994) 1382.