Conformational Composition of Propanol in Gaseous State and in Matrix Isolation

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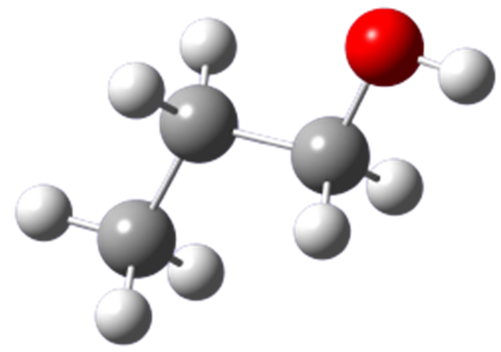
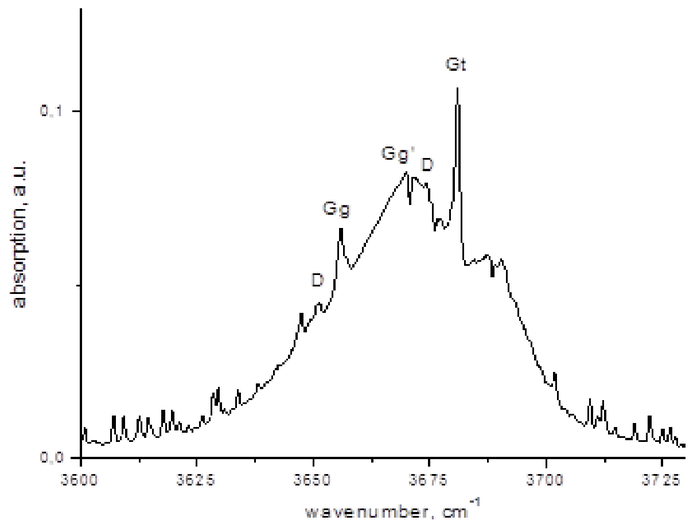
Introduction

Molecules of monohydric alcohols can form different cluster structures due to hydrogen bonding. Moreover, each molecule of alcohol with more than one atom of carbon can be found in different conformations, which are formed as a result of rotation of atoms around chemical bonds. In the case of propanol (structural formula CH_2-CH_3-CH_3-OH), the molecule of which has two structural dihedrals, nine stable configurations exist: one plane structure and four pairs of enantiomers (or mirror-image pairs). Since enantiomers have similar energy and optical properties, the difference between them is usually neglected. As a rule, propanol conformers are designated by a symbolic title using a generally accepted scheme of dihedral angles CCCO+CCOH via big + small letters for trans- (T, t), gauche- (G, g) and gauche'- (G', g') conformers.

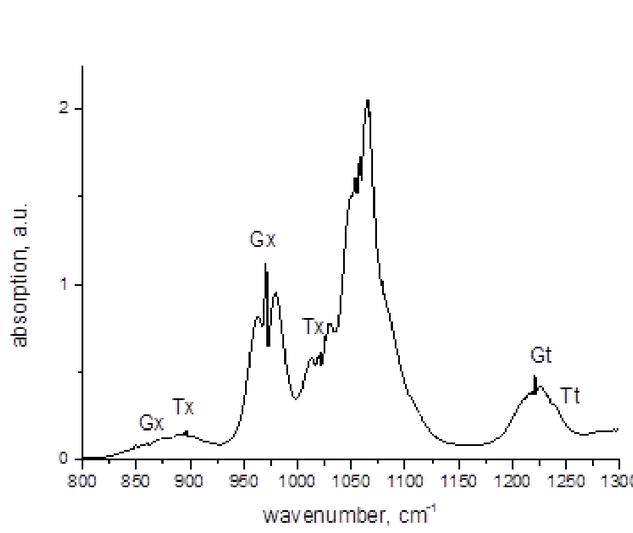


Tt conformer of propanol molecule

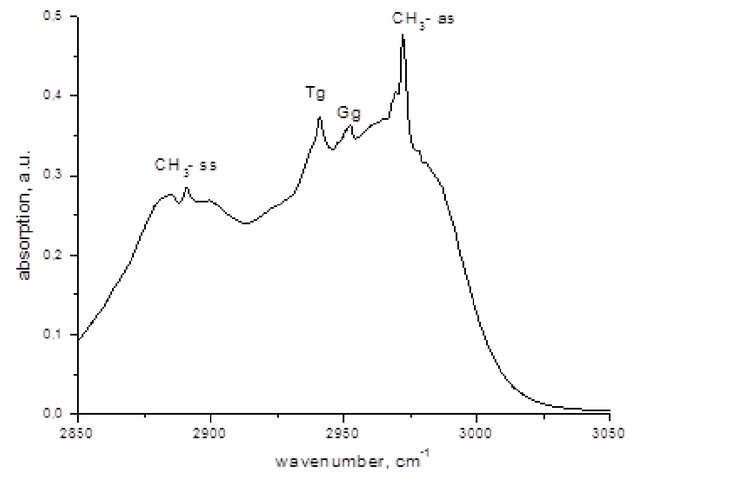
Conformational analysis of gaseous propanol



IR absorption band of gaseous propanol corresponding to the stretching vibrations of free OH groups

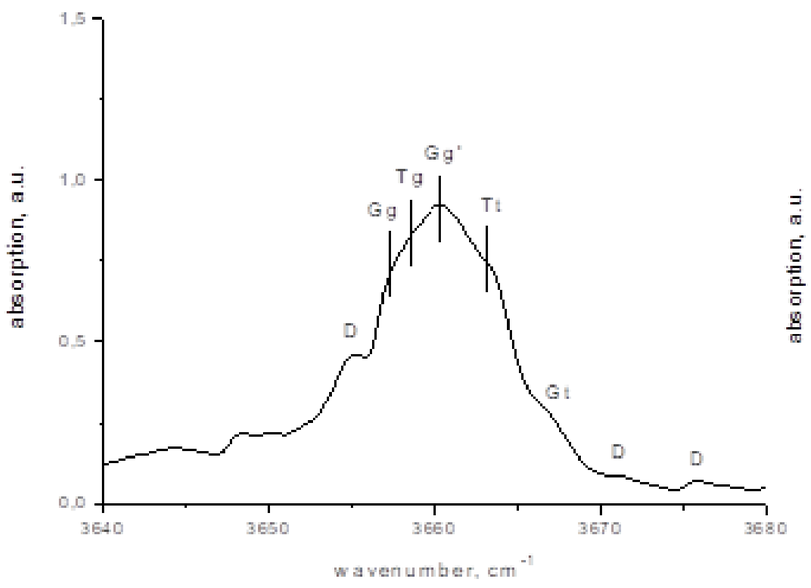


FTIR spectrum of gaseous propanol in the range 800 – 1300 cm^{-1}

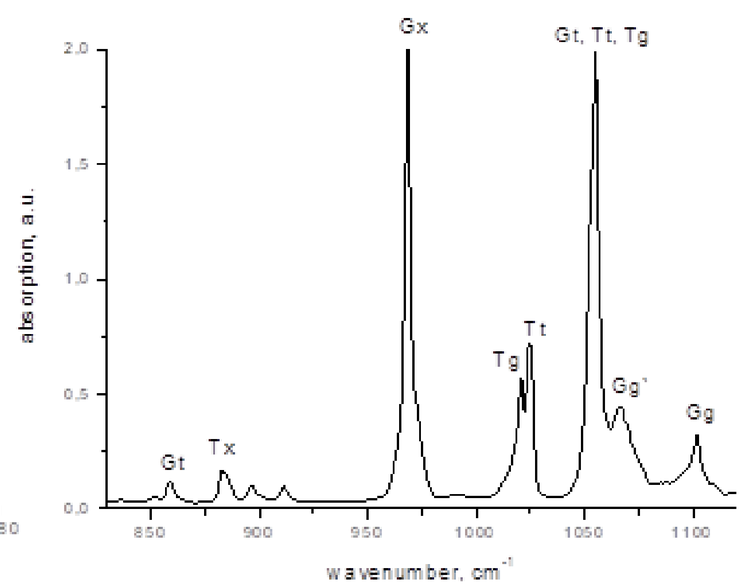


FTIR spectrum of gaseous propanol in the region of the stretching C – H vibrations

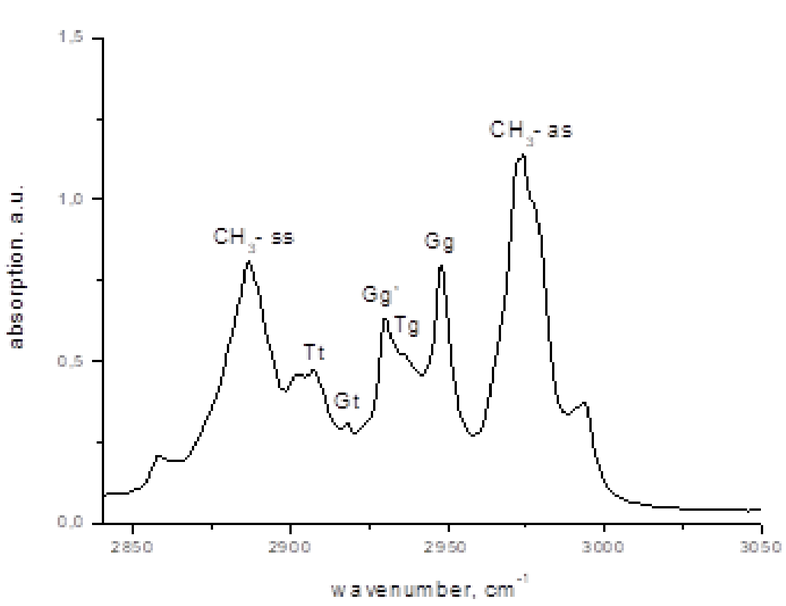
Conformational analysis of propanol in matrix isolation



IR absorption spectrum of propanol isolated in an argon matrix at 35 K in the region of OH stretching vibrations



IR absorption spectrum of propanol trapped in an Ar matrix at 20 K in the spectral region 830 – 1120 cm^{-1}



IR spectrum of propanol trapped in an Ar matrix at 20 K in the spectral region of stretching C – H vibrations

Conformational analysis of the experimentally recorded IR absorption spectra of propanol in gaseous state and in a low-temperature argon matrix, carried out for different spectral ranges, showed that the conformational composition of the samples in these two cases is different.

Thus, the results of our studies show that gaseous propanol contains the largest number of Gt conformers, which are the most stable of the five possible propanol conformers according to a number of quantum mechanical calculations. The propanol molecules isolated in a low-temperature argon matrix are influenced by the environment; therefore, in this case the most energetically favorable form is Tg conformer, which prevails in percentage.