Quantum-Chemical Study of Conformational Properties of Propanol

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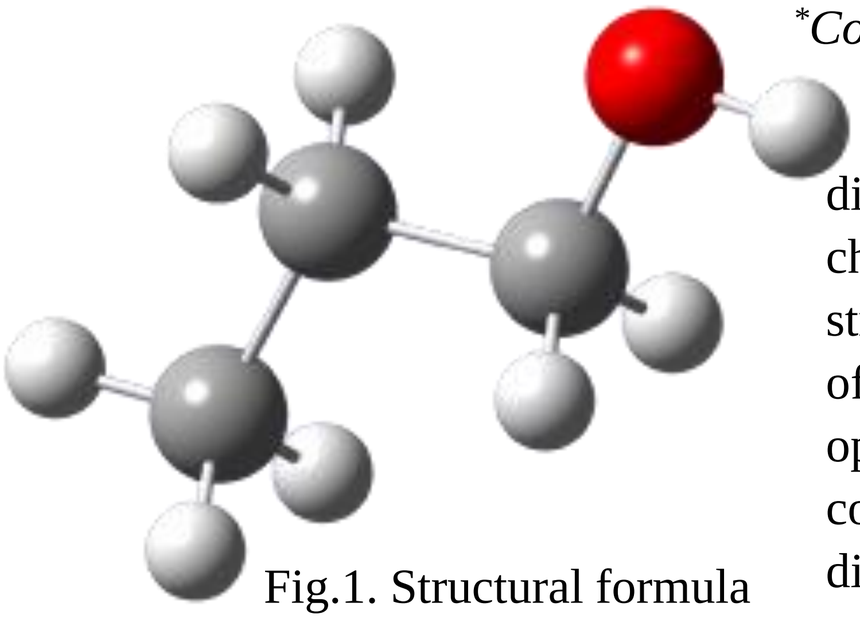

Fig.1. Structural formula n-propanol (CH_2-CH_3-CH_3-OH).

Molecules of monohydric alcohols with more than one carbon atom can be found in different conformations, which are formed as a result of rotation of atoms around chemical bonds. In the case of n-propanol (Fig.1), 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.

Table 1

Quantum-chemical calculations of optimal geometry, dipole moments, energy of five propanol conformers were made at DFT: B3LYP/cc-pVTZ level of theory.

Conformer	Tt	Tg	Gt	Gg′	Gg
Dipole moment, D	1,43	1,64	1,47	1,61	1,59
Energy E, hartree	-194,433735	-194,433884	-194,433833	-194,433699	-194,433958
Energy E, kJ/mol	-510 582,988	-510 583,379	-510 583,245	-510 582,893	-510 583,574
ΔE, kJ/mol	0,586	0,195	0,329	0,681	0

It is determined that Gt conformer is the most probable configuration (having the lowest energy), but energies of other conformers differ by not more than 1 kJ/mol.

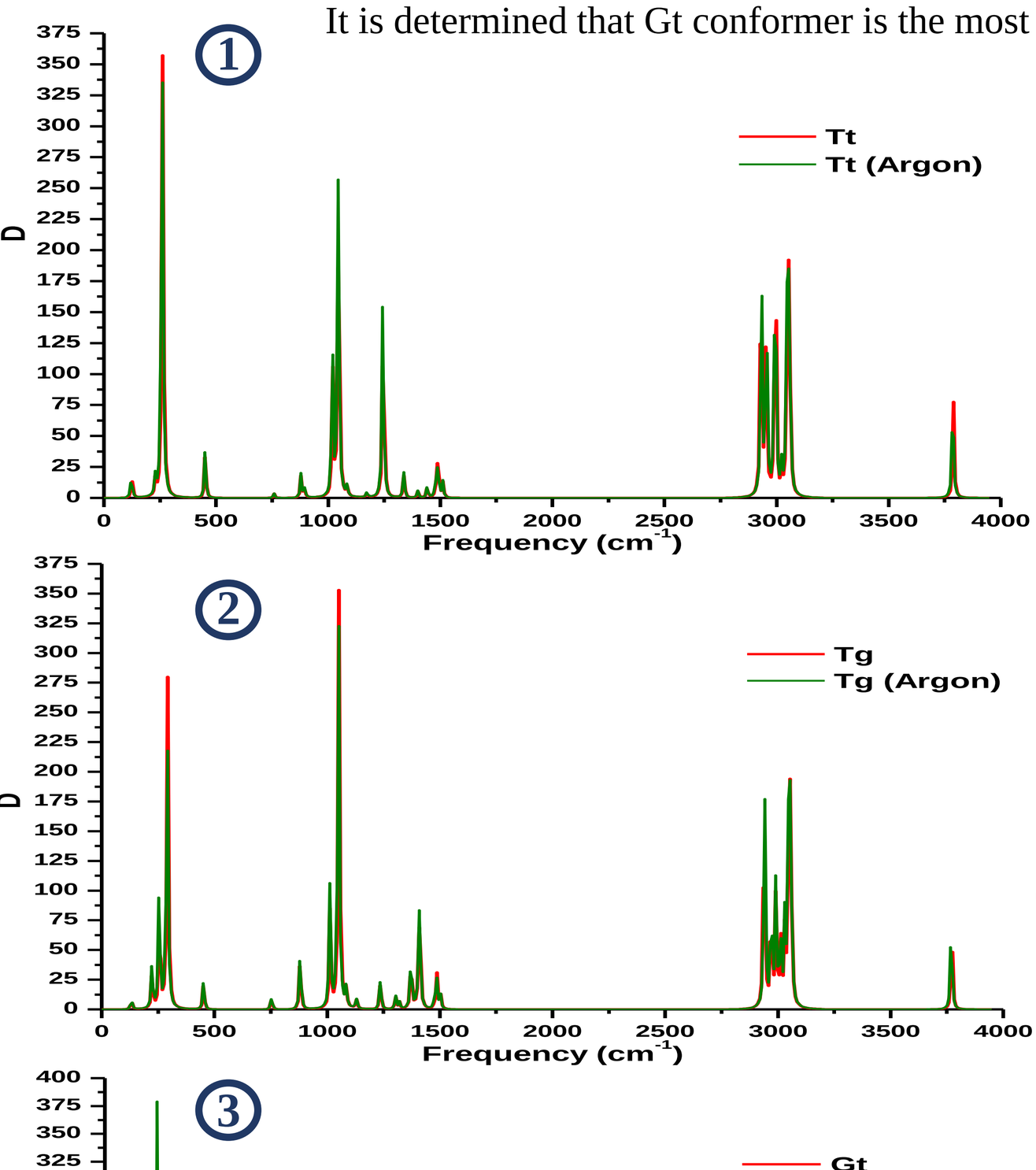

Fig. 2. IR spectra of five propanol conformers in vacuum and argon environment: 1 - Tt conformer; 2 - Tg conformer; 3 - Gt conformer; 4 – Gg conformer; 5 – Gg' conformer.

Similar calculations were made for n-propanol molecules in argon environment (Fig.2) in order to use their results for the interpretation of experimental IR spectra of propanol in matrix isolation.