PROGRAMME UTILIZATION OF MOLECULAR SPECTROSCOPY METHODS AT THE ORGANIC COMPOUNDS INVESTIGATION

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The proposed component of the system of program use of methods of molecular spectroscopy combines the results of many-year systematic studies in the field of experimental and theoretical vibrational spectroscopy of carbohydrates and of empirical simulation of IR spectra of organic compounds with the use of the data base "spectrum — fragmentary composition of a compound" and is designed for solving two kinds of problems:

1. Identification and analysis of an unknown compound.
2. Analysis of the spectroscopic and structural properties of a particular compound.

The given component of the system consists of two parts: an information-retrieval subsystem containing computer catalogs of spectral information and a computer subsystem including the required software. Its block-diagram is given below.

In analyzing an unknown compound, the system’s capacity is used to the full. With the aid of database on IR spectra and structural formulas of ~ 32000 organic compounds, empirical simulation of the spectrum of an unknown compound is carried out and its possible structures are generated. Next, for the most probable structure of the unknown compound, complete theoretical analysis of the IR spectrum of the established compound in both its isolated state and with regard to its molecular surrounding is carried out. This analysis includes the calculation of:

1) the frequencies, forms, potential energy distributions of normal vibrations;
2) the Cartesian displacements of atoms from equilibrium positions;
3) the electronic structure;
4) absolute integrated intensities of the IR absorption bands.

The method for calculating the spectrum is chosen depending on the complexity of the structure of the compound and the character of its spectrum. Two approaches are realized in the system: the classical approach based on the valence-optical theory and a combined approach that combines the classical analysis of the frequencies and forms of normal vibrations and a quantum-chemical evaluation of intensities.

The proper choice of the calculation technique largely predetermines the success of the investigation. For carbohydrates, the combined approach has proved to be quite efficient.

Potentialities of the system are demonstrated by an example of a whole number of derivatives of glucopyranosides.