PROGRAMME UTILIZATION OF MOLECULAR SPECTROSCOPY METHODS AT THE ORGANIC COMPOUNDS INVESTIGATION

R. G. ZHBANKOV[a], M. V. KOROLEVICH[a], B. G. DERENDYAEV[б], V. N. PIOTTUKH-PELETSKY[б]

[a] B.I.Stepanov Institute of Physics, NAS of Belarus, 70, Skorina ave., 220072 Minsk, Belarus; e -mail: zhbankov@dragon.bas-net.by

[б] N.N.Vorozhtsov Institute of Organic Chemistry, Siberian Branch of the RAS, 9, Acad. Lavrentiyev ave., 630090 Novosibirsk, Russia; e-mail: der@nioch.nsc.ru

Abstract

Computer system is proposed of program use of methods of molecular spectroscopy, which 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.

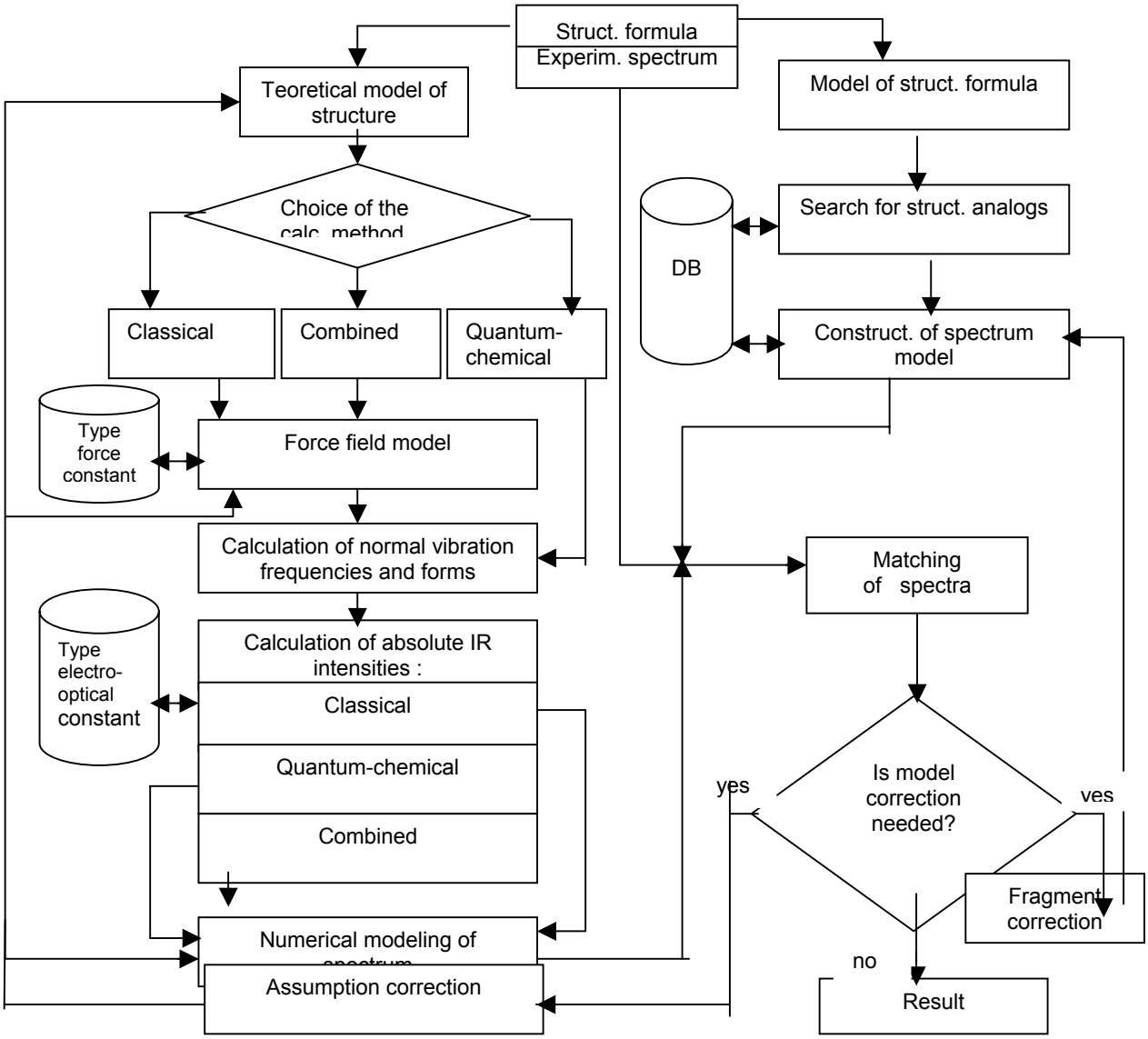
Key words: IR spectra; Data Base; Normal coordinate analysis; Absolute IR intensities;

1.Introduction

The rapid development of various directions of spectroscopy, of its scientific grounds, and technical base is accompanied by an ever increasing gap between the extremely high potentialities of spectroscopic methods and their wide practical use. Identification of molecular spectra and extraction of a maximum of information contained in them require a great deal of preparatory work, mastering of the theoretical and experimental fundamentals of the spectroscopic method used, detailed study of the specificity of the spectra of the class of compounds under consideration, analysis of the spectra of various model substances, involvement of calculations of conformations and spectra of molecules or their fragments. Investigation of the spectra of particular classes of compounds calls for special methodological procedures and approaches, whose neglect can lead to a considerable depletion of obtained information and frequently - to insufficiently substantiated and erroneous conclusions.
The solution of this problem, as we see it, is in the development of ad hoc analytical-reference software for the methods of molecular spectroscopy. Such an approach, which provides quick, purposeful use of the methods of molecular spectroscopy for solving concrete scientific or practical problems, called program use of molecular spectroscopy methods (PUMSM) was proposed in a monograph [1].
This global, extremely urgent problem includes at least two main tasks:
1) application of concrete spectroscopic methods (their combination) for studying the specific structural and chemical characteristics of individual classes of organic compounds;
2) use of the potentialities of concrete spectroscopic methods for analyzing the presence of certain structural fragments in the molecules of diverse organic compounds (including compounds with an unknown structure) and construction of model spectra.

2. Results and discussion

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 (DB) "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 subsistem containing computer catalogs of spectral information and a computer subsistem 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 data base 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 [2-3]. 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 [4-5]. 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 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 [6-8].

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

4. Conclusions

The program-purposeful application of methods of molecular spectroscopy based on a combination of empirical and theoretical simulation of vibrational spectra enables a significant increase in the efficiency of spectroscopic studies of the structure and properties of various classes of organic compounds.

References

[1] R.G.Zhbankov, P.V.Kozlov, Physics of Cellulose and its Derivatives, Nauka i Tekhnika, Minsk, 1983(in Russian).
[2] V. N. Piottukh-Peletsky, I. K. Korobeinicheva, T. F. Bogdanova, S. G. Molodtsov, B. G. Derendyaev, Anal. Chim. Acta, 409 (2000) 181.
[3] V. N. Piottukh-Peletsky, B. G. Derendyaev, R.G.Zhbankov, M.V.Korolevich, Zh. Prikl. Spectrosk., 68 (2001) 532.
[4] M.V. Korolevich, Calculation and analysis of absorption bands intensities in the IR spectra of some types of carbohydrates, Ph.D. dissertation, BSSR Academy of Sciences, Minsk, 1987.
[5] M.V. Korolevich and R.G. Zhbankov, in P.Carmona, R.Navarro and A.Hernanz (Eds.), Spectroscopy of Biological Molecules: Moderm Trends (Proc. 7-th European Conference on the Spectroscopy of Biological Molecules), Kluwer Academic Publishers, Dordrecht, 1997,pp.569-570.
[6] M.V. Korolevich, J. Mol. Struct. (Theochem), 306 (1994) 261.
[7] M.V. Korolevich and R.G. Zhbankov, J. Mol. Struct., 440 (1998) 247.
[8] M.V.Korolevich, R.G.Zhbankov, J. Mol. Struct., 556 (2000) 157.