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MATHEMATICAL MODELING OF CHEMICAL-TECHNOLOGICAL PROCESSES

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ABSTRACT

The article describes the mathematical modeling of chemical-technological processes and the scientific-methodological processes carried out in this regard.

Keywords: simulation, experimental, invention, mathematical, chemical-technological.

INTRODUCTION

With the development of computing technology, based on the application of quantum mechanics in chemistry, it can be noted that today the computer has become a research tool for conducting primary chemical or physical experiments.

Today, the field of science named "Computer chemistry" is not limited to quantum-chemical calculations and includes a wide range of theoretical methods, including various non-empirical and semi-empirical methods of calculating the physico-chemical properties of matter, artificial intelligence and neural networks. Application of methods, database, statistical characteristics of chemical processes and covered the dynamics. Each of the mentioned directions can be the subject of a university course. This means that chemical students studying at universities have the skills to predict the properties and reactivity of substances, to develop ways of synthesizing chemical compounds with certain properties based on the study of the relationships between the structure and properties of substances. Is very important in formation.

The textbook on "Mathematical modeling of the structure and properties of chemical compounds" is written on the basis of the program approved by the Ministry of Higher and Secondary Special Education of the Republic of Uzbekistan. Aimed at students and the main focus is on visualizing the spatial structure of the molecule; methods based on classical mechanics for calculating the statistical characteristics and dynamics of the molecular geometric structure; molecular mechanics, molecular dynamics, Brownian dynamics, Monte Carlo method; semiempirical methods of quantum-chemical calculations; non-empirical (ab initio) methods of quantum-chemical calculations; The course focuses on theoretical knowledge of structure-property correlations (QSAR) and practical exercises in ChemOffice, HyperChem and GAUSSIAN universal software packages.

MAIN PART:

The main topics of chemical modeling are the following.

- use of computers in chemical research;
- Molecular modeling techniques using force fields;
- Quantum chemistry in the analysis of molecular systems.
- Studying molecular structures using quantum-chemical methods;
- Solving chemical problems using semi-empirical methods;
- Ah initio non-empirical quantum chemical calculation methods;

- Solving problems in ab initio quantum chemical calculation methods;
- properties and electronic structure of chemical compounds;

QSAR and QSPR analysis in clinical and pharmaceutical research.

- The use of methods. Key skills to be learned from the course:
- spatial view of the molecular structure;

Prediction of physico-chemical properties of organic compounds based on their chemical structure and management of database systems of chemical compounds:

1. Quantum chemistry;
2. classical mechanics: molecular mechanics, molecular dynamics, Brownian dynamics, geometrical structure of molecules based on Monte Carlo methods, methods of calculating statistical and dynamic characteristics.

The main focus in studying the course is not only on the theoretical foundation of the issue, but also on their practical application. Computer software plays an important role in performing these tasks.

It is known that, on the one hand, various software packages for working with text and graphics (Microsoft Office, ABBYY Fine- Reader. Adobe Reader, WinDjView, Adobe Photoshop, CorelDRAW, ACDSee, Origin, etc.), on the other hand, to perform complex calculations used and specialized programs that facilitate the visualization of objects, as well as in the implementation of substance identification programs that are used and incorporate the parameters of various substances (ChemDraw, Isis/Draw, ChemBio-Draw, HyperChem 6.0, Atomic Models v1.0, MOPAC, GAUSSIAN, etc.) are used. Software designed to work with equipment intended for research (NMR-, IR-spectrometers, illuminating and scanning electron microscopes, chromatographs, chromato-mass spectrometers, etc.) are also specialized programs.

The development of electronic computing technology allowed researchers of various fields to perform calculations that could not be calculated "by hand". This created conditions for more accurate and qualitative research of the investigated phenomena.

The use of quantum-chemical theories to calculate the structure and properties of molecular systems requires high-speed computing. In solving such issues Used for these purposes, except for powerful EHMs Downloadable software also plays an important role.

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The use of quantum-chemical theories to calculate the structure and properties of molecular systems requires high-speed computing. In addition to powerful EHMs, the software used for these purposes also plays an important role in solving such problems. Among the currently available software packages, the following can be distinguished: GAMESS, Gaussian, Dalton and NWChem software packages, HyperChem, Chem Oficce, PRIRODA.

GAMESS program (Program GAMESS)

General Atomic and Molecular Electronic Structure System is a general system for calculating atomic and molecular structures. There are currently three versions of GAMESS, which are supported and updated in the United States (US), England (UK) and Russia (PC). The main

distinctive advantage of GAMESS-PC is its high speed compared to other quantum chemical programs. This is very important in the investigation of complex molecules. But today, the most functional (but slow) version is GAMESS-US.

Some of the capabilities of the GAMESS program are listed below:

1) It is possible to calculate the molecular wave function in the RHF, UHF, ROHF, GVB and MCSCF approximations by the coherent field method;
2) The perturbation theory based on the clusters and functional density (the theory of perturbations) takes into account the electron correlation energy based on the conformational interaction.
3) MNDO, AMI and PM3 semi-empirical methods have the possibility to perform calculations;
4) Optimizing the molecular geometry using analytical gradients and automating the transition state search;
5) Solving vibration problems has the ability to calculate the frequencies of valence vibrations of IR and combined scattering spectra;
6) Analysis of position according to dipole moment, electrostatic potential, electron and spin density, Mulliken and Lovdin Is able to calculate molecular properties such as;
7) It is possible to model the effect of the solvent.

GAUSSIAN program (Program GAUSSIAN)

Currently, the Gaussian software package is one of the most widely used tools for performing quantum chemical calculations. The main reason for this is that it incorporates many quantum-chemical techniques, has high efficiency, and is user-friendly.

The main capabilities of the G98 and G03 software complex:

1) Energy calculation and structure optimization of the investigated system in molecular mechanics, semi-empirical approximations, bounded and unbounded Hartree-Fock methods;
2) Calculation of energy with analytical gradients for multi-configurational methods in which the correlation energy is widely used: perturbation theory, connected clusters, configurational interactions, density functional mutual agreement and there is an opportunity to optimize the structure;
3) prof. Developed by Morokuma et al. molecular partitioning methodology - ONIOM allows for modeling even very large molecular systems. According to it, molecular systems are divided into 3 areas. They consider the full level of calculation accuracy;
4) analytically calculates force constants for RHF, UHF, DFT, RMP2, UMP2 and CASSCF methods;
5) It is possible to calculate a wide range of molecular spectra, including thermochemical parameters and Nuclear Magnetic Resonance (NMR) chemical shifts;
6) It takes into account the influence of the solvent on the properties of the system being tested.

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