MODERN SCIENTIFIC TENDENCIES
OF USING COMPUTER EXPERIMENTS IN CHEMISTRY

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Modern computer modeling in chemistry is known, to aim at simulation of properties and reactivity of chemical compounds and molecular dynamics. Some computer models have such accuracy level which can be compared with one of modern chemical experiments. First of all, these are calculations of some molecular structures and spectrums and intermolecular methods of quantum chemistry and theoretical molecular spectroscopy. One also should mention problems of chemical equilibrium and chemical kinetics modeling, mathematical processing of measurement readings in some problematical cases, issues of optimum experiment planning.

Development of numerical methods of solving equations of theories of many particles enables to model and predict properties of solids, liquids, solutions, to calculate characteristics of processes on surfaces, to evaluate parameters of molecular systems, instilled inside framework complexes, inert or reaction matrices, to perform simulation in the study of materials.

The process of proceeding from structures to reaction molecular dynamics, that is, to modeling elementary chemical reactions is very problematical even for a small number of atoms in the system. Numerical solution of quantum mechanical equations, describing molecular collisions followed by redistribution of their constituent particles, that is, chemical reactions is possible only for the simplest processes, for instance, for interacting atoms with diatomic molecules. Substantial success has been achieved in the process of applying semiclassical approximation, according to which nuclei move lengthwise classical trajectories, determined by the given surface of all system potential energy.

Constructing potential energy surfaces (PES) is a major integral part of computer experiment in chemistry, which may be time-consuming (some weeks or even months) for modern computers. The common scheme of mathematical model is the following [1]. First, stationary points, that is, coordinates of minimums, maximums and saddle points should be found on the potential energy surfaces. In order to consider the existence of a stable molecule or molecular complex, on the potential surface of the main electron state there should be minimum, whose energy is less than one of any other fragments the molecule can be divided into. If there are several minimums, it is possible for a molecule to have several isomers. Nuclei coordinates answering to minimum points, determine equilibrium geometrical configurations, while energies in respect to corresponding limits of dissociation into constituent parts specify energies of chemical system bonds. The determination of the positions and energies of the saddle points is necessary for evaluation of energies activation while considering elementary chemical reactions. The existence of minimums with the energy above the dissociation limit shows the possibility of intermediates formation in the reaction molecular system. Calculating the differences of electron energies of various electron states for those nuclei geometrical configurations which answer to minimum points, one can interpret or predict electron spectrums of molecules.

After approximation of potential surface fragments in the neighborhood of minimum points one can forecast fluctuating and revolving spectrums. Found a set of electron fluctuating and revolving energies of molecule one can calculate using formulas of statistic thermodynamics, any thermodynamics functions of a given substance. When considering the molecular system where particles redistribution occurs, that is, chemical reaction, the section of potential energy along the movement of the least energy, combining reagents and products is calculated and then the constant of elementary chemical reaction rate is evaluated. The program of actions described realizes the model of calculations of substance properties without considering any empirical data.

The potential energy surface, which in quantum chemical models is calculated directly, in molecular mechanics is approximated by empirical functions of a certain extent of complexity, such as, for instance, sums of pair potentials of atom interactions. These potential functions determining so-called molecular force field, contain some parameters whose numerical value is selected in the optimum in order to meet requirements of both calculated and experimental characteristics of a molecule. In the simplest case these parameters are equilibrium bond lengths and valence angles and also hardness coefficients of elastic forces, connecting atomic pairs. This method is based upon assumption of possibility of transferring these parameters from one molecule to another, thus numerical values of parameters found for some elementary molecules, are used further for predicting properties of more complex compounds.

Due to molecular mechanics, using PC of even low capacities one can analyze structures of large polyatomic molecules for some reasonable time.

When modeling with the help of molecular dynamics methods or Monte-Carlo method, the property involved of the system of a large number of molecules is calculated through statistic averages of positions and motions of molecules. As in molecular mechanics methods, it is necessary to enumerate all particles of the system and to set potentials of particle interactions. However, unlike molecular mechanics in the approaches mentioned the areas of setting particle potentials of interaction should be extensive enough. This fact places exacting demands upon the ways and methods of potential calculations.

Practically all equations, connecting molecular parameters and substance properties, that is, macroscopic properties, are solved numerically and efficiency of their solving substantially depends upon the capacity of a computer used.

One can mention the examples of successful Monte-Carlo method and molecular dynamics method application for modeling equilibrium compositions of mixtures at the constant pressure, phase equilibrium, adsorption at the surface of solids, liquids properties in micropores. The number of particles when being modeled by the Monte-Carlo methods and molecular dynamics methods this the help of modern generation computer system may reach its maximum.

The problems of searching for stable turning isomers of polymer molecules which are extremely important for biochemical application are also solved by these methods.

The most difficult stage is numerical solving equations of quantum theory of collision with the account of particles redistribution, that is, the most important stage for chemistry. Even with the help super computer systems, the results obtained by the present day look like classical chemistry book examples: $\mathbf{D + H_2 \rightarrow HD + H}$ or $\mathbf{O + H_2 \rightarrow OH + H}$.

Moreover, modern experimental methods of molecular dynamics investigation enable to measure partial constants of rate and directly to compare experimental and theoretical results. Simpler, and, as a result, more practical methods of calculating rates of chemical reactions are usually found when simplifying a complete quantum model [3].

Modern computer systems with high performance and storage capacities enable to find and estimate a great number of possible variants of one or another compound synthesis and to choose the optimum plan of this synthesis. Computer synthesis is considered to be an extremely perspective trend in organic chemistry [2]. The performance of any program of computer synthesis starts with putting in some initial data about the structure of a given chemical system.

The well-known programs of computer synthesis, such as SYNGEN (J. Hendrixon, the USA), EROS (J. Gasteiger, FRG), SYNCHEM (G. Gelernter, the USA) store tables (or matrices) of atoms bonds and information about free electrons on the external valence shell of every atom. Of particular interest is the program COMPASS (N.S. Zefirov, D.L. Lushnikov, E.V. Gordeeva), based on the combination of exclusively combinatorial methods and empirical rules of retrosynthetic analysis.

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