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Use of programs to determine the physicochemical parameters of compounds and products

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Today, quantum chemistry makes it possible to accurately calculate equilibrium internuclear distances and valent angles, barriers of internal rotation, formation energy and dissociation energy, frequencies and transition probabilities under the influence of electromagnetic radiation in a very wide wavelength range (from X-ray electron spectra to NMR spectra), activation energy, cross sections and rate constants of the simplest chemical reactions. It plays a decisive role in obtaining information about intermolecular interactions, when developing models of the influence of the medium on a molecule. At present, quantum chemical approaches to describing the evolution of chemical systems, in particular, the evolution of excited molecules after exposure to a different external field, are developing rapidly. Also important is the role of quantum chemistry in the study of high-molecular compounds in the construction of models in molecular biology and quantum pharmacology, as well as in chemical materials science. Quantum-chemical theory and experiment, mutually complementing and correcting each other, contribute to a significant acceleration and depth of research in chemistry, biology, physics, materials science and other areas of natural science. Computational chemistry is a relatively young field of chemistry, which arose at the intersection of chemistry and computer technology, based on the application of graph theory to chemical problems of fundamental and applied nature. In the future, when creating quantum supercomputers, science will not have difficulty in evaluating even the most complex processes.