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An Introduction to Computational Chemistry

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Chemistry is the branch of science which contemplates compositions, structures, and properties of substances. It also studies the chemical transformations of atoms and molecules along with the energy involved in such processes. Although, most of these analyses rely on practical experiments performed by the learner, 'theoretical chemistry'—a subfield of chemistry based on the combination of mathematical calculations and physical laws—is also used in many cases. The process of incorporating well developed theoretical mathematical models of chemistry into efficient computer programs and calculating the structure and properties of substances is known as computational chemistry. It uses computer simulations to assist in solving chemical problems and generating data complementary to experimental data. It applies laws of physics to understand the molecular nature of substances.

Computational chemistry investigates fundamental properties of atoms, molecules, and chemical processes. The ones studied mostly are

- molecular geometry (the shapes of molecules)—bond lengths, bond angles
- electronic structures—potential energy surfaces
- molecular and transitions state energies—heat of reactions, energy of activation
- chemical reactivities- prediction of nucleophilic and electrophilic sites, determination of rates of reaction
- spectral data—IR, UV, and NMR
- substrate-enzyme interaction—active site determination
- physical properties of substances—strength, melting point based on arrangement of atoms or molecules in the particular substance.

All these calculations are performed with certain 'tools' or methods. The main tools used in computational chemistry are molecular mechanics, Ab Initio calculations and semiempirical calculations. Molecular mechanics is based on classical physics where the behavior of atoms and molecules can be explained by considering the molecule as a collection of balls (atoms) held together by springs (bonds). Knowledge of bond lengths and energies is used to calculate the energy of a particular molecule and optimize its geometry. This method is fast and hence good when computer resources are limited. This method needs experimental data for calculation parameters and is suitable for large molecular systems and processes, with no breaking or forming of bonds. Ab Initio (Latin for "from the start") calculation is an implication of quantum physics where Schrodinger equation is solved for a molecule to give its energy and wavefunction. This method uses approximation in the calculation, does not depend on experimental data, has a scope of use in a broad range of molecules, is slow and is expensive due to requirement of computers with the latest configuration. Semiempirical calculations are also based on Schrodinger equation, but also uses experimental values. Hence, the mixing of experimental values with mathematical equations makes this method 'semiempirical' and gives it a speed lesser than molecular mechanics but higher than Ab Initio calculations. It is generally used for medium-sized molecular systems. There are two

more methods: Molecular dynamic calculations which applies the law of motions to molecules; and Density function calculations[1] relatively which is a new method based on Schrodinger equation. Nature of molecule under investigation guides the choice of method.

Computational chemistry has a vast application in several fields: materials sciences[2] where it is used to calculate and determine properties of various substances like conductors, semiconductors, ceramics, plastics; pharmaceutical sciences where a molecule can be docked into the active site of an enzyme to see how it fits; new drug development research[3] where quantitative structure-activity relations can be established between a medicinally active molecule and its three-dimensional structure using steric and electric molecular descriptors, the molecular model thus obtained can be used to identify potential 'pharmaceutically active' molecules; synthetic chemistry where identification and characterization of reaction pathways[4] along with the most likely products can help to devise new cost-effective synthetic pathways.

The practice of computational chemistry has seen a definite advent in last few years which is because of ability to—generate crucial data before experimenting; minimize waste generation during chemical reactions; and determine some properties which are otherwise difficult or costly to obtain experimentally. There are some limitations as well that arise due to the absence of real chemical environments like solvent and temperature effects, vibrational corrections, and other intermolecular effects. Computational chemistry is not a replacement of actual experiments, but surely enables chemists to explain and rationalize known phenomena and explore new or unknown chemical processes.

[1]https://www.sciencedirect.com/science/article/pii/S0927025619306147

[2]https://www.researchgate.net/publication/298908570_Computational_materials_design_of_crystalline_solids

[3]https://www.researchgate.net/publication/330462660_Molecular_Modeling_in_Drug_Design

[4]https://www.pnas.org/content/114/29/7555