Study of Enzyme interaction theory, dielectric, electrostatic and spatial constants of Carbonium ion in Lysosome

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Abstract

Studying the chemical interaction in solution and enzymes indicate a wonderful success due to the expansion and complexity of these systems. The MM energy reticular areas but they can't face electronic motivated states with chemical phenomena which include bond forming and breaking. The combination and quantum and molecular mechanics in which the small part of system (for example solute) is reviewed by quantum mechanics and the remains by MM, provides a powerful tool for studying interaction and structure.
A general method to detailed study of enzyme interaction is shown. This method is considered a full complex of applied enzyme with the solution around it. It is also reviewed all the different quantum and classic factors of energy which can affect interaction. These factors include mechanical quantum energy which related to the split of bond, re-distribution of applied component, spatial classic energies and electrostatic reactions between applied component and enzyme. The electrostatic polarization of enzyme atoms and moment direction of environmental water molecules are simulated by microscopic dielectric model. The resulted soluble energy from the polarization is considerable and must be configured in any real calculation of chemical interaction which includes everything beyond on isolated atomic space. Without the ionization of acidity group, the bond distribution on applied component won't be logical. The same dielectric model can be used to review applied component interaction in solubilisation. In this case, the solubilisation and interaction can be compared.
In this article, I study the middle form constancy of Carbonium ion in glycoside bond breaking by lissome. It is found that the electrostatic constants are in important factor in increasing interaction step rate which resulted in forming Carbonium middle ion. It seems that spatial factors such as applied component pressure on Lysosome bond have less importance.

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