

# An Exploration of Computational Software in Organic Chemistry teaching

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**Abstract:** Organic chemistry is an important course for students majoring in chemical engineering. The knowledge such as molecular orbitals, reaction mechanism and stereochemistry, etc. are the key and the difficult points. The model demonstration or simple animation simulation in traditional teaching cannot reveal the chemical reaction process in essence and also cannot really solve poor spatial imagination of students. In recent years, with the emergence of more and more quantum chemistry software, computational chemistry has shown its strong application advantage in organic chemistry teaching. In this paper, Gaussian software is introduced to assist teaching. Introduction of computational chemistry can make students understand stereochemistry, reaction and molecular orbitals deeply; and also, a new way to learn organic chemistry is offered.

**Keywords:** Organic chemistry teaching, computational chemistry, teaching exploration

## 1. Introduction

Organic Chemistry is an important and basic course for chemical engineering, pharmacy, biology, materials and other related majors. It mainly consists of four parts: nomenclature, structure, reaction and synthesis of organic compounds. Among them, three-dimensional structure and chemical reaction are the key points and difficulties in teaching and studying organic chemistry. Comprehensive understanding and application of reaction mechanism have always been the focus and difficulty of organic chemistry teaching and learning. For many years, it is widely believed that this part is abstruse; the knowledge is messy and irregular to follow. For students, how to understand correctly the relationship between stereochemistry of organic compounds and reaction mechanism is the key to learn organic chemistry well. And this is exactly the weak spot of students because they don't have enough imagination for spatial structure. They are always confused about the changes in the three-dimensional structure of the reaction and the relationship between the major products and the reaction conditions. On the other hand, organic chemistry teaching is faced with a greatest dilemma now is that teaching hours are compressed seriously. Thus, how to improve efficiencies have always been the major objectives in teaching and learning.

The model demonstration and animation simulation in traditional teaching cannot touch the essence of reaction and also cannot really solve poor spatial imagination of students. Recently, with the popularity of computers and the software of quantum chemistry, application of computational chemistry in organic chemistry teaching especially in the teaching of organic reaction mechanism is gradually becoming a trend [1-6]. Computational chemistry can be used to build the three-dimensional structure of organic molecules, construct molecular orbitals, demonstrate infrared spectroscopy dynamically, calculate molecular energy and the energy of reaction process, and track reaction process and so on. Therefore, computational chemistry can simplify some abstract chemistry problems, so as to reduce the difficulty of teaching and enhance students' interest in learning organic chemistry. At the same time, it also provides ideas for students to solve practical problems by using computational chemistry.

Based on the above teaching ideas, computational chemistry is introduced into organic chemistry teaching. In this paper, we only introduce application of Gaussian software in organic chemistry.

## 2. Application examples in organic chemistry

### 2.1 Studying on nucleophilic substitution reaction mechanism

Nucleophilic substitution is one of important reactions of alkyl halide. It can be second-order or first-order substitution. Reaction of sodium iodide with methyl bromide is a typical second-order substitution reaction.

In the reaction, nucleophile I<sup>-</sup> attacks the central carbon atom from the backside of C-Br bond. This reaction is a concerted reaction, taking place in a single step with C-Br bonds breaking and C-I forming at the same time. Reaction undergoes a transition state with C-I bond partially forming and C-Br bond partially breaking. Three-dimensional structure of the transition state is presented clearly by computational software and the process of iodide anion attacking and bromine anion leaving can be visibly observed through the dynamic demonstration by clicking on “start animation” button (Figure 1).

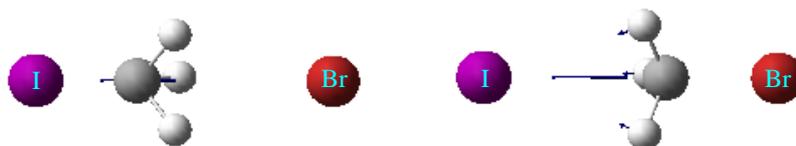


Figure. 1 Visualization of I-C-Br vibration in transition state.

The transition state involves a five coordinated carbon atom with two C-Br and C-I partial bonds. It can be concluded that transition state must behave as high energy because five-coordinated carbon is an unstable state. In the transition state, the negative charge (red) is delocalized over the iodide and bromide. And then, the negative charge will leave with the Br<sup>-</sup> anion (Figure 2).

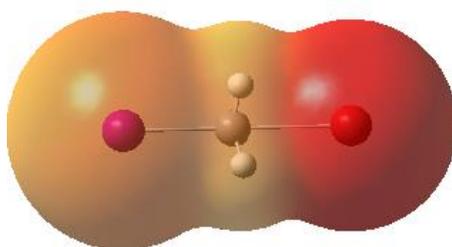


Figure. 2 Electrostatic potential surface of transition state. Red in map represents negative cloud.

### 2.2 Visualization of molecular orbitals

Molecular orbital is another key point in organic chemistry study. The drawing and interpretation of molecular orbital pattern is an important method to understand the chemical bonds and the physical and chemical properties of organic molecules. However, it is difficult to understand because of its complexity. For example, it is well known that benzene is a flat ring, each carbon atom is sp<sup>2</sup> hybridized and all unhybridized p orbitals are parallel to each other and overlap to form a delocalized  $\pi$  orbital like sandwich. From Figure 3, it can be seen that electron cloud is centered along each carbon atom on benzene, and thus it is concluded that each carbon atom has the same probability to react with electrophile. That is, visualization can help us understand molecular orbitals deeply.

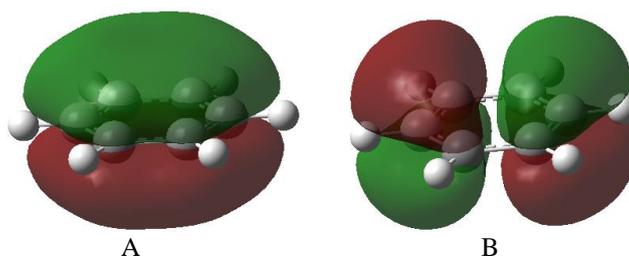


Figure. 3 Visualization of molecular orbitals of benzene. A) delocalized  $\pi$  orbital of benzene, B) HOMO orbital of benzene.

### 2.3 Animation of infrared spectroscopy

Infrared spectroscopy is one of the most important methods to determine organic structure by observing the vibrations of covalent bonds and providing evidence for the functional groups present in molecule. Simple simulation of vibration can help students understand various vibration modes attached to functional groups. For example, in propenal, several vibrations are important to determine groups present in molecule: double-bonded C-H bonds, carbonyl C=O bond and carbonyl C-H bond. All of these vibrations can be simulated by clicking on “start animation” button as presented in Figure 4. Visual simulations cannot only make us understand easily, simplify complex issues, but also can enhance students’ interest in learning organic chemistry.

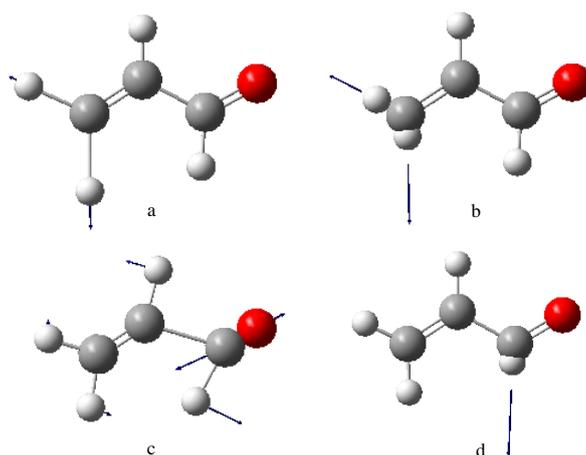


Figure. 4 Animation of Infrared Spectra of propenal. a) and b) Stretching vibrations of two double bonded C-H around  $3150\text{ cm}^{-1}$ , c) The carbonyl C=O stretching vibrations around  $1720\text{ cm}^{-1}$ , d). Stretching vibration of carbonyl C-H bond around  $2890\text{ cm}^{-1}$ .

### 2.4 Other applications in organic chemistry teaching

In addition to visualization of molecular orbital and animation of Infrared Spectra, computational chemistry can also be used to calculate molecular energy, dipole moment, electrostatic potential surface and other important parameters and also can be used to track reaction process.

## 3. Conclusion

Applications of computational chemistry in organic chemistry teaching can not only reduce the difficulty of students' learning, but also increase their interests in organic chemistry. At the same time, it also provides ideas for students to solve practical problems by using computational chemistry. Therefore, computational chemistry as an auxiliary means of organic chemistry teaching will attract more and more attention.

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