Interactive Animation of Chemical Reactions Based on Quantum Chemical Calculations -Computer Microscope 2002-

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Abstract
CG animations of chemical reactions based on quantum chemical calculations were produced. The reactions include hydration of CO₂, SO₃, N₂O₄, and phthalic anhydride. User-interface of the animation was studied.

1. Introduction

We have produced CG animations of chemical reactions based on quantum chemical calculations. We call these animations the “Computer Microscope”[1]. The Computer Microscope is an effective tool for better understanding how and why chemical reactions occur. As a useful teaching material, however, the Computer Microscope needs to be more user-friendly and appealing. We have revised the original animations to interactive animations of chemical reactions, the “Computer Microscope 2002”, that gives students the chance and means of molecular manipulation.

2. Method

In this work, the ab initio calculation software, Gaussian 98W (Gaussian, Inc.), was used to find the transition states and the reaction path of chemical reactions according to the intrinsic reaction coordinate (IRC) theory[2]. The calculations were then used for such reactions as hydration of CO₂, SO₃, N₂O₄, phthalic anhydride and others. The Quick Time (Apple Computer, Inc.) movie was produced by DIRECTOR 8.5J (Macromedia, Inc.) following the display of bond order or molecular orbital of the structure in the each reaction stage which was drawn by CAChe MOPAC (Fujitsu, Inc.). Quick Time VR Authoring Studio (Apple Computer, Inc.) was used for the production of the three-dimensional (3D) rotation.

3. Features of the Computer Microscope 2002

The introduction section of the Computer Microscope has been revised to explain the basics of reaction path studies. The goal of the revision is to help students understand the reaction profile. To explain the reaction profile, the reaction path of a simple reaction such as chlorine molecule attacked by a hydrogen atom is shown on a 3D potential energy surface. The most probable pathway is demonstrated by the movement of a ball along the steepest fall line from a transition state on the potential surface. Theoretically, the reaction profile shown by the most probable pathway representing the relation between potential energy and IRC is obtained and used for various complex reactions.

![Figure 1 The reaction profile of the reaction of hydrogen atom and chlorine molecule](image)
for the movie is placed just under the reaction profile to allow the student to move the reaction back and forth along the IRC with a computer mouse. This type of “virtual hands-on” experience helps students look into the process of chemical reactions.

The updated version includes a transition state search simulator. This is a trial-and-error simulator in which students select initial configurations and orientations of the reactants for given molecules. Correct choices lead to the next step, while incorrect choices bring the students back to the beginning. Finding the true transition state and reaction path give students basic information about reaction path studies based on quantum chemical calculation.

The 3D display of the chemical change is shown by two viewpoints; Top view and Side view of the CG animation of the reaction process. Thus it is easy to see that a reactant approaches a substrate from a certain direction and with a specific orientation to produce a product(s). The approaching route and molecular orientation should help the student understand the chemical change on the basis of atomic orbital. The QT-VR allows the student to rotate the molecules of the reactant, transition state, and product. The rotating HOMO and LUMO combinations also help the student understand which atomic orbital plays an important role in bond formation and scission.

4. Conclusion

The CG animations of chemical reactions based on quantum chemical calculations were produced which gives students the chance and means of molecular manipulation.

An English version of “Computer Microscope 2002” is available on CD-ROM. For enquiries, please contact Akira Ikuo at: ikuo@u-gakugei.ac.jp

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