An Approach to the Electronic Textbook of Basic Chemistry Linking Chemical Experiments

CG Teaching Materials based on Quantum Chemical Calculation

Akira Ikuo, Yusuke Yoshinaga and Haruo Ogawa
Department of Chemistry, Tokyo Gakugei University, Tokyo 184-8501, Japan

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Abstract: We tried to make CG teaching materials toward electronic textbook of basic chemistry linking chemical experiment for university student. The CG teaching materials could demonstrate the nature of the reaction such as structural change by ball-and-stick model or space filling model with electrostatic potential, and potential energy change by the reaction profile. The materials included 1) formation of di-atomic molecule such as hydrogen iodide, 2) hydroxylation of methyl chloride as a model of Walden's inversion. These CG teaching materials enabled to load with desktop, laptop, tablet computer, and smart phone. The CG teaching material of hydroxylation of methyl chloride was tried to combine with chemical experiments to make electronic textbook of basic chemistry.

1 INTRODUCTION

Chemistry is the subject that has been studied through the experiment. Understanding the observed phenomena, chemists use to imagine and explain observations in terms of molecules. Observed phenomena and molecular-level models are then represented in terms of mathematics and chemical equation. These three thinking levels of observable level, symbolic level, and molecular level, respectively was mentioned (Tasker and Dalton, 2010). Visualization is great help for students to have images of phenomena, chemical concepts, and molecular world. It is our aim to produce computer graphics (CG) teaching material, which provides realizable images of the nature of chemical reaction (Ikuo et al., 2006).

The reaction of simple molecule such as hydrogen halide and related compounds plays a fundamental role in the development of chemical kinetics and theoretical chemistry (Allison et al., 1995; Eyring and Polanyi, 1913; Sullivan, 1962). The reaction of equation (1) is often used for explanation of reaction rate and

$$I + H_2 \rightarrow HI + H \quad (1)$$

chemical equilibrium in "Chemistry II" of Japanese high school (Sanseido, 2004). Generally, reaction profile is used to represent relationship between potential energies (PE) and reaction coordinate. The profile is often used in high school chemistry textbooks (Daiichigakusyusya, 2004; Jikkyosyuppan, 2004; Keirinkan, 2003; Sanseido, 2004; Tokyosyoseki, 2004). It is sometimes difficult for student to realize the meaning of reaction coordinate in the profile because of the representation by a diagram of PE surface in two-dimensions (PE-2D) except the rare case of rough sketch of analogues in three-dimensions (PE-3D) in physical chemistry textbook of university (Atkins and Paula, 2002; Moor, 1982). Also images of synchronization with successive changes of the structure of objective molecules and distribution of electrical character can provide clear images of the reaction.

We developed CG teaching material based on quantum chemical calculation of chemical reaction for university student, which can be used to desktop, laptop, and tablet computer, as well as smart phone. This paper introduces our works of CG visualization of fundamental chemical reactions for realizing certain images of the reaction mechanism and an approach to the electronic textbook of basic chemistry linking chemical experiments, which integrates the observable level experiment and the molecular world.

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2 PROCEDURE

2.1 Quantum Chemical Calculation

The semi-empirical molecular orbital calculation software MOPAC (Stewart, 1989a, b, 1991) with AM1, PM3, and PM5 Hamiltonians in CAChe Work System for Windows (ver. 6.01, FUJITSU, Inc.) was used in all of calculations (Ikuo et al., 2009) for optimization of geometry, for search of potential energies of various geometries of intermediates, for search of transition state, and search of the reaction path from the reactants to the products via the transition state. The optimized structure of the transition state was verified by the observation of a single absorption peak in the imaginary number by the use of the program Force in MOPAC (Stewart, 1989a, b, 1991) for vibration analysis. If the peak was observed, Intrinsic Reaction Coordinate (IRC) (Fukui, 1970) calculation was done and the reaction path was confirmed.

2.2 CG Teaching Material

A movie of the reaction path was produced by the software DIRECTOR (ver. 8.5.1J, Macromedia, Inc.) or Flash CS4 software (Adobe, Inc.) following the display of the bond order of the structure of the reactants in each reaction stage, which was drawn by the CAChe. It was confirmed that the Cast members were arranged on the stage and the molecular models of reactants moves smoothly. The ball was arranged on the reaction profile and the movement of the ball and the reactants was confirmed. The movie file was converted to the Quick Time movie by the Quick Time PRO (ver. 7.66, Apple, Inc.) and was saved to iPad (Apple, Inc.) by using the iTunes (ver. 10.7, Apple, Inc.).

2.3 Practice of Teaching Material

Teaching material was practiced to the first year students of teacher training course for elementary school and the second year students of natural environmental science course, of “Chemistry laboratory” at Tokyo Gakugei University. Teaching material used for the trial was the CG movie shown by the tablet computer.

3 RESULTS AND DISCUSSION

3.1 $I + H_2 \rightarrow Hi + H$

The CG teaching material of rearrangement by collision of diatomic molecule and one atom as shown in equation (1) was developed. PE of 2-D and 3-D is shown in figure 1. The figure clearly shows these changes of PEs with display on PE surface in 3-D, which offers a bird-eye view of the reaction profile. Two Valleys of lower energies and hilltop on the transition state at the saddle point can be recognized boldly. Possible pathways of the reaction from the reactants of I and H_2 to the products of HI and H *via* the transition state at saddle point can be readily traced. The CG teaching material is able to provide information about change of the PE and structure of reactants in a certain state simultaneously.

The electrostatic potential on electron density (EPED) model and ball-and-stick model of the intermediate, I-H-H, and the reaction profile were combined in the left side of figure 1 for easier recognition of those three. The electrostatic potential (Kahn et al., 1986) was calculated based on the coordinates of atoms from the IRC calculation (Fukui, 1970) and superimposed on to the iso-surface of the electron density at the value of 0.01 e $Å^{-3}$ as shown in the upper left part of the CG. The values of electrostatic potentials were represented in different colour on the model of intermediate. The model by EPED provides information about electrostatic distribution of the intermediate with realistic shape on the way of the reaction. In the middle of the CG, skeletal structure in the ball-and-stick model in which diameter of the stick reflects calculated bond order is shown. The lower left part of the CG shows the reaction profile, which demonstrates the degree of the reaction progress by the ball indicating the PE versus the reaction coordinate. Student could correlate this reaction profile with the reaction path in the right side of CG. The left side of the CG is able to provide information about characteristics of intermediate of molecule in a certain state on the progress of reaction.

From the posteriori survey, number of correct answers in question about “Energy” increased 28% compared with the preliminary survey (n=49). Students described their comments in the free description section of the questionnaire, such as,“With image, it was easier for me to understand the way of reaction and changes of energy.” and “I could see that reaction mechanism and energy

change is closely related." These comments suggest that many students were able to obtain the concept of energy change in chemical reaction from the CG teaching material.

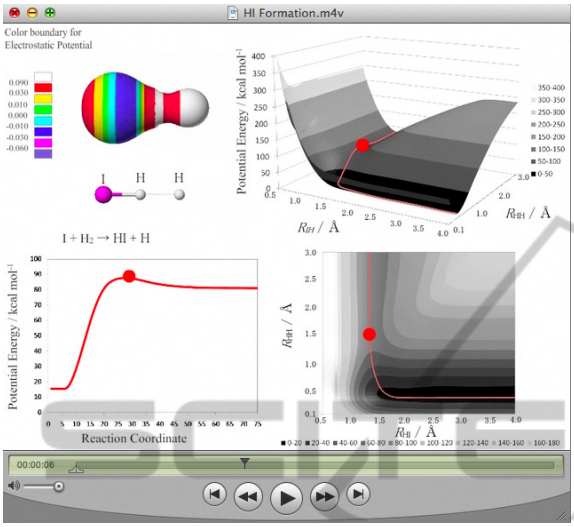
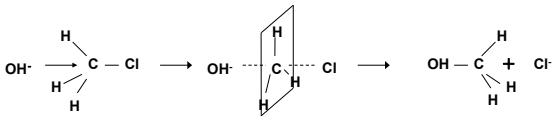


Figure 1: CG teaching material of $I + H_2 \rightarrow HI + H$.

3.2 $OH^- + CH_3Cl \rightarrow CH_3OH + Cl^-$

Structural change of reactants in the reaction shown in equation (2) was studied as a model of Walden's inversion, which is also shown in scheme 1.

$$OH^- + CH_3Cl \rightarrow CH_3OH + Cl^- \quad (2)$$



Scheme 1: Images of Walden's inversion.

Reaction of hydroxide and chloromethane is a typical example of the Nucleophilic Substitution in the 2nd order reaction. Carbon atom at the centre to which halogen attaches is attacked by the nucleophile, hydroxide, from a position 180 degrees from chlorine and then methyl alcohol forms. Therefore, the transition state was searched from the reactants where the bond angle of O-C-Cl was adjusted to 180°.

The inter-atomic distances of C-Cl in CH_3Cl was calculated as 1.87 Å (1.87 Å) (Weast, 1982), and C-O in CH_3OH was 1.41 Å (1.43 Å) (Shida, 1981). These values were in good agreement with the literature values in the parentheses. Energy between the initial state of reactants and the final state of products was 165.01 $kJmol^{-1}$. The value was in fairly good agreement with literature (Shida, 1981) value of 162.90 $kJ\ mol^{-1}$.

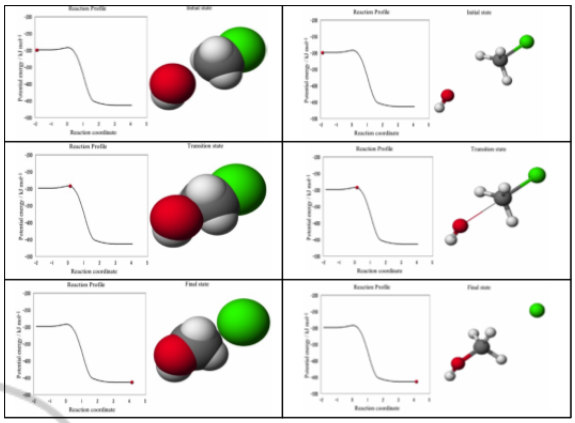


Figure 2: Selected picture of CG movies: from the CG teaching material; Reaction profile and image of reactants; in space filling and ball-and-stick model.

Selected picture of CG movies are shown in the figure 2. The CG shows the reaction profile, which demonstrates the degree of the reaction progress by the ball indicating the potential energy versus the reaction coordinate. Movies were made by using not only the space filling model which shows realistic shape but also the ball-and-stick model which shows change in molecular configuration easily. A student is expected to obtain the image of an umbrella reverse like motion in Walden's inversion. In the space filling, the existence probability of the electron is 90 %. In the ball-and-stick, the thickness of stick changes by bond order.

When the CG is touched by student, the Quick Time control bar appears and the red ball can move by student's choice. This manual control feature provides "Hands-on" feeling to student. This CG teaching material could provide not only images of energy change during reaction but also images of dynamical structure change during chemical reaction.

The CG teaching material could demonstrate the structural change of reactants with both space filling and ball-and-stick models along with the reaction profile, which can provide image of energy change during the reaction.

From the result of the questionnaires (n=103), the answer judged to be able to acquire the image of Walden's inversion (the image to which an umbrella reverses) was follows; the image obtained from the reaction formula was 24% and from the CG teaching material was 51%. The number of CG teaching material was better than that of the reaction formula. Students were abele to obtain the image of drastic change of the structure in Walden's inversion from the CG teaching material.

The CG teaching material can be loaded with note PC, tablet PC, and smart phone.

We tried to produce electric textbook for chemical laboratory (Figure 3), which integrates the observable level experiment and the molecular world.

Figure 3: Prototype electronic textbook.

4 CONCLUSIONS

We produced CG teaching materials included 1) formation of di-atomic molecule such as hydrogen iodide, 2) hydroxylation of methyl chloride as a model of Walden's inversion. These teaching materials could demonstrate the nature of the reaction such as structural change by ball-and-stick model or space filling model with electrostatic potential, and potential energy change by the reaction profile. The CG teaching materials enabled to load with note PC, tablet PC, and smart phone. The CG teaching material of hydroxylation of methyl chloride was tried to combine with chemical experiments to make electronic textbook of basic chemistry.

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