Development of Electronic Textbook for Chemical Experiment
Taking Esterification as an Example

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Abstract: Developing policy of electronic textbook for chemical experiment of student's laboratory at the university was decided which aimed at integration of observable level experiment and the molecular world. The developed textbook could display picture of apparatus and flow-chart of small-scale experiment in addition to CG teaching material. The CG teaching material in the textbook effectively demonstrates images of dynamical reaction mechanism. Students were able to conduct experiment smoothly and safely with the electronic textbook inserted in the Ziploc type plastic bag.

1 INTRODUCTION

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 (Gilbert, 2009 and Tasker, 2010). Student's difficulties and misconceptions in chemistry are from inadequate or inaccurate models at the molecular level (Kleinman, 1987). A molecular structure visualized by the computer graphics (CG) provides a deeper understanding of molecular structure (Tuvi-Arad, 2006).

It is our aim to produce a CG teaching material based on quantum chemical calculations, which provides realizable images of the nature of chemical reaction (Ikuo, 2006 and 2009). Molecular level animations combined with video clips of macroscopic phenomena enabled students to predict the outcome better (Velazquez-Marcano, 2004). If the CG teaching material is combined with chemical experiments of student's laboratory, students would observe the reaction from three thinking levels, namely, phenomena in the actual observable level and CG teaching material in the molecular level, and chemical equation in the symbolic level.

The CG teaching material on the tablet computer was effective to provide image of "Energy" change and also effective to provide image of "Structure" change and "Migration of Electron" during chemical reaction (Ikuo, 2012). Our ultimate goal is to produce an electronic textbook linking chemical experiment, which integrates these three levels.

This paper introduces our works of CG visualization of fundamental chemical reactions for realizing certain images of the reaction mechanism and development of the electronic textbook for chemical experiment of student's laboratory at the university, which integrates the observable level experiment and the molecular world of the esterification.

2 DEVELOPMENT OF ELECTRONIC TEXTBOOK

2.1 Policy

Flow chart of development of the electronic textbook for chemical experiment is shown in the Scheme 1. Reaction was selected based on importance in fundamental chemistry. To exhibit phenomena, experimental condition was optimized for the student laboratory and experimental program was made. For easier understanding of experimental procedure, enlargeable-photos and flow charts were used in addition to regular text-base description. The electronic textbook could acts as an individual electronic tutor. To provide image of molecular world, computer graphics (CG) images such as realistic shape of molecules, CG teaching material (movie) were made based on quantum chemistry

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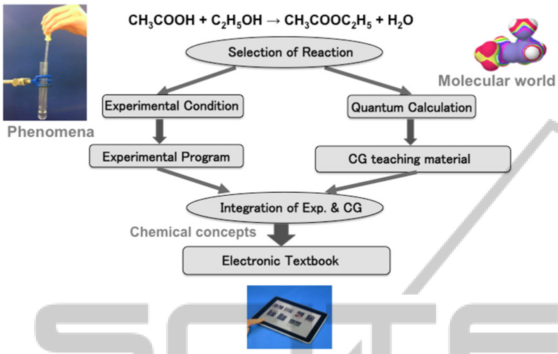
calculation. Students would be able to see structure and energy change during reaction while they are watching actual reaction progress. In this manner, observable level experiment and the molecular world could be integrated. In order to use the electronic textbook on the lab bench, it need to be covered with a waterproof, Zip-lock type, case.



Scheme 1: Flow chart of developing method.

2.2 Method

2.2.1 Quantum Chemical Calculation

Structures of intermediates on reactions and their electrostatic potentials on electron density were calculated as follows: the semi-empirical molecular orbital calculation software MOPAC (Stewart, 1989) with AM1, PM3, and PM5 Hamiltonian in the CAChe Work System for Windows (Former name of SCIGRESS, ver. 6.01, FUJITSU, Inc.) was used in all of calculations for optimization of geometry by the Eigenvector Following method, for search of transition state by use of the program with Saddle point Search, and for search of the reaction path from the reactants to the products via the transition state by the intrinsic reaction coordinate (IRC) calculation (Fukui, 1970). Details of procedure of the quantum chemical calculations were described in the previous paper (Ikuo et al., 2006). The electrostatic potential on electron density (EPED) (Kahn, 1986) was calculated based on structures from the results of the IRC calculation.

2.2.2 CG Teaching Material and Electronic Textbook

A movie of the reaction path was produced by the software DIRECTOR (ver. 8.5.1J, Macromedia, Inc.) following the display of the bond order of the structure of the reactants in each reaction stage, which was drawn by the CAChe. The obtained CG of EPED model was combined with those of ball-and-stick model and reaction profile in the same reaction stage. It was confirmed that the drawn CGs of the molecular models of reactants moves smoothly. The green ball, which indicates progress of the reaction, was arranged on the reaction profile and simultaneous movements of the ball and the reactants were confirmed. Created movie file was converted to the Quick Time movie for iPad by the Quick Time PRO (ver. 7.66, Apple, Inc.). Electric textbook was produced with iBooks Author (ver. 2.1.1, Apple, Inc.) and was saved to iPad (Apple, Inc.) by using the iTunes (ver. 11.2.1, Apple, Inc.).

3 ELECTRONIC TEXTBOOK

3.1 Contents of Electronic Textbook

3.1.1 Reactions

Formation of HF: The CG teaching material of rearrangement by collision of diatomic molecule and

$$F + HCl \rightarrow HF + Cl \tag{1}$$

one atom as shown in equation (1) was developed. Potential energy (PE) of 2-D and 3-D is shown in the 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 F and HCl to the products of HF and Cl *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.

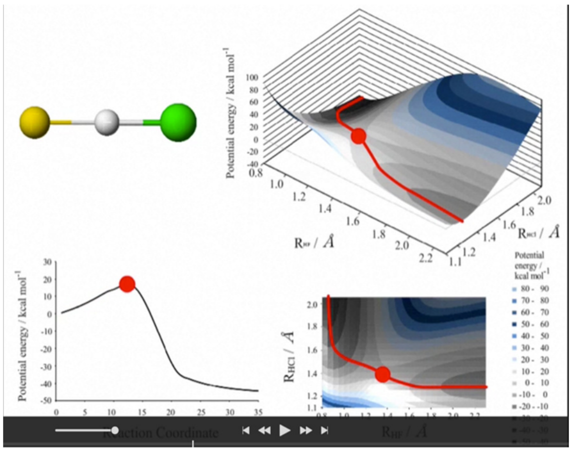
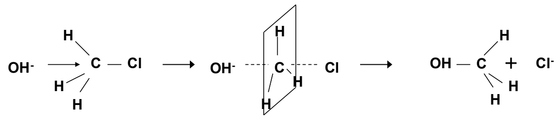


Figure 1: CG teaching material of HF formation.

Walden's inversion: Structural change of reactants in the reaction, shown in the Scheme 2, was studied as a model of Walden's inversion.



Scheme 2: 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.
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 *vs*. the reaction coordinate. Movies were made by using not only the ball-and-stick model, which shows change in molecular configuration easily, but also the space-filling model, which shows realistic shape. A student is expected to obtain the image of an umbrella reverse like motion in Walden's inversion.

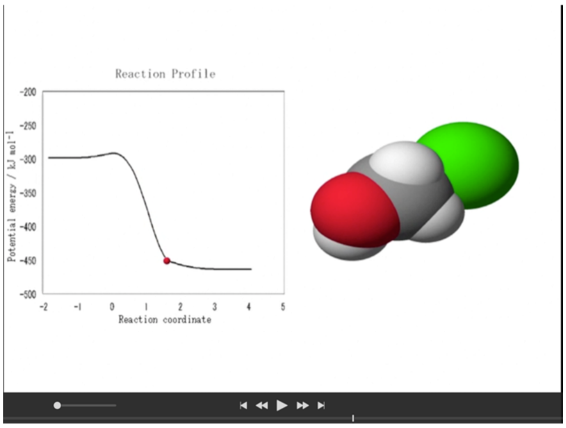


Figure 2: CG teaching material of Walden's inversion.

Nitration of Benzene: A picture of teaching material is shown in the Figure 3. Left part of the material shows the reaction profile, potential energy *vs*. reaction coordinate, which indicates the degree of the reaction progress by the red ball on the profile. Right part shows structural change shown in ball and stick model, While choreographed animation of chemical reaction are common (For example, Tasker & Dalton, 2010), CG based on theory in the present study could provide not only images of energy change but also images of dynamical structure change with more realistic shape.

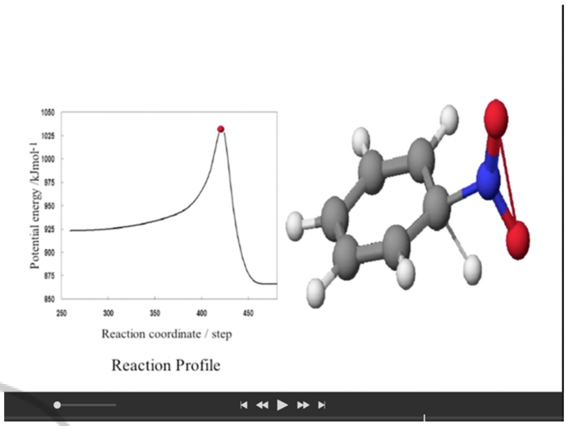
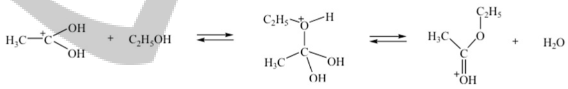


Figure 3: CG teaching material of benzene nitration.

Esterification of Ethanol and Acetic Acid: The mechanism of esterification of acetic acid and ethyl alcohol the reaction is well known (For example Loudon, 1984), and generally, the esterification proceeds in the presence of proton catalyst. The rate-determining step includes the paths of an attack of the oxygen atom of hydroxyl group of ethyl alcohol to the central carbon of the formed carbonium ion and release of water as shown in the Scheme 3. This step dominates all over the reaction.



Scheme 3: Mechanism of esterification on the rate-determining step.

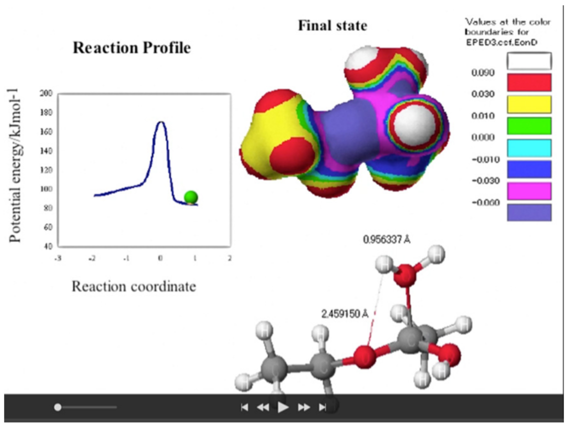


Figure 4: CG teaching material of esterification.

The Figure 4 shows the combination CGs on the way from the state of reactants to that of products *via* the transition state. The teaching material demonstrates the changes of electrostatic potential and realistic shape of the intermediate of the reaction on the reaction profile in all stages at the same time.

Distribution of the electrostatic potential among the intermediate can be seen by the colours. The model by electrostatic potential provides information about electrostatic distribution of the intermediate on the way of the reaction.

3.1.2 Feature of Electronic Textbook

The CG teaching material of the esterification was combined with chemical experiments of student's laboratory for the purpose of making electronic textbook of basic chemistry to provide experiment at the observable-level, CG visualization at the molecular-level, and chemical equation at the symbolic-level.

The electronic textbook was inserted with images of experimental procedure in the flow charts and photographs, which can be enlarged by students touch (Figure 5). Student can write memo for the observation. CG teaching materials of reaction profiles were also inserted (Figure 6). When student touches the CG teaching material in the tablet computer, the teaching material appears to show image of the structural change during the reaction. Student can compare different reaction mechanisms. If student touches the material again, the Quick Time control bar appears and the green ball on the profile can move by student's choice. Student can manipulate the reaction back and forth until they obtain the image of the reaction.

Students were able to conduct experiment smoothly and safely with the electronic textbook inserted in the Ziploc type plastic bag (Figure 7).

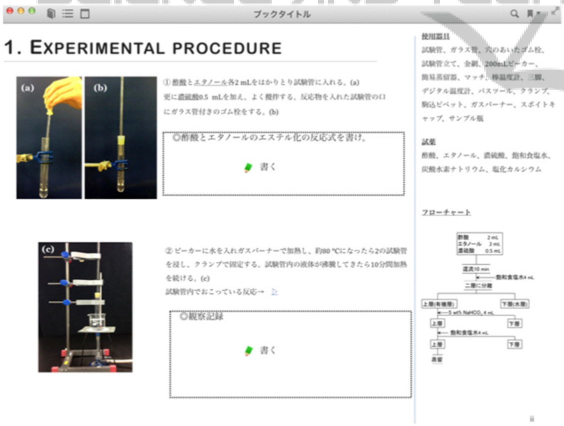


Figure 5: Experimental procedure in electronic textbook.

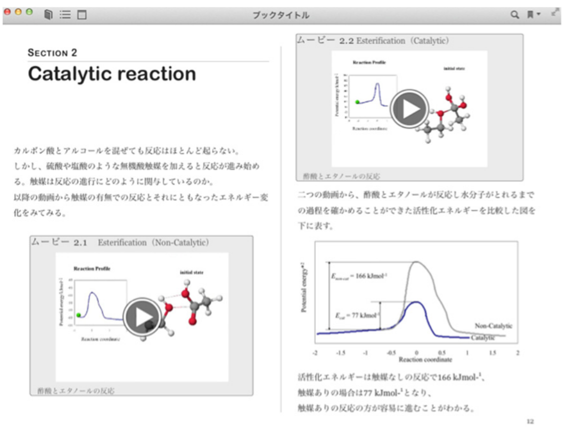


Figure 6: CG teaching material in electronic textbook.

Figure 7: Electronic textbook with waterproof cover.

4 CONCLUSIONS

Developing policy of electronic textbook for chemical experiment of student's laboratory at the university was decided which aimed at integration of observable level experiment and the molecular world. The electronic textbook was developed according to the policy. The developed textbook could display picture of apparatus and flow-chart of small-scale experiment in addition to CG teaching material. The CG teaching material in the textbook effectively demonstrates images of dynamical reaction mechanism. From the preliminary study, students were able to conduct experiment smoothly and safely with the electronic textbook inserted in the Ziploc type plastic bag. The developed electronic textbook could be used to integrate the observable level experiment and the molecular world.

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