Use of Tablet in College Chemistry Experiment

- An approach to developing an electronic textbook -

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***Abstract*—We are developing an electronic textbook for a basic chemistry-experiment for university students in which reaction mechanisms are shown by Computer Graphics (CG). The CG of chemical reaction was made based on empirical molecular orbital calculations. The CG included following reactions as a model of Walden's inversion where drastic change in structure takes place; hydroxylation of methyl chloride, formation of 2-butyl alcohol and 1-butyl bromide. The CG can simultaneously demonstrate the nature of the reaction such as structural change by the space-filling and ball-and-stick models in addition to providing an image of energy change by the reaction profile. The electronic textbook also displays pictures of apparatus and flow-charts of small-scale experiments. Therefore, students are able to conduct experiments smoothly and safely while studying dynamical reaction mechanism shown by the CG. The electronic textbook on a tablet could be used to integrate the experimental observable level and the molecular world.**

Keywords-Computer graphics; Visualization; Reaction mechanism; Electronic textbook; Chemical experiment.

I. INTRODUCTION

In order to understand the observed phenomena, chemists imagine and explain observations in terms of molecules. Observed phenomena and molecular level models are then represented in terms of mathematics and chemical equations [1], [2]. Student's difficulties and misconceptions in chemistry are from inadequate or inaccurate models at the molecular level [3]. A molecular structure visualized by the computer graphics (CG) provides a deeper understanding of a molecule [4].

It is our aim to produce a CG teaching material based on quantum chemistry calculations, which provides realizable images of the nature of a chemical reaction [5], [6]. We have reported that the CG on tablet was effective to provide images of chemical reaction, such as, "Energy" change, "Structure" change and "Migration of Electron" [7]. If the CG is linked with textbook for college chemistry-experiment, students could observe the reaction from the three thinking levels [1], [2], namely, phenomena in the observable level, the CG in the molecular level, and chemical equation in the symbolic level. Our ultimate goal is to produce an electronic textbook of chemistry experiment, which integrates these three thinking levels.

An electronic textbook has several advantages over the paper textbook. For example, realistic images can be shown by photograph, movie and CG. These images may include experimental procedures, molecular structures and reaction mechanisms. In addition, programmable capability [8], hyper-link and networking features provide interactive operation. Many electronic textbooks of chemistry exist, but most of them are almost identical to the paper book, and very few are related to the chemical experiment [9]. Moreover, tablet applications, which include CG movie of reaction mechanism related to student laboratory experiments, are not available.

In Section II of the paper, an approach to developing an electronic textbook for college chemistry-experiment, which tries to integrate the observable level experiment and the molecular world, is described. In Section III, the features of the proposed textbook are described. We conclude in Section IV.

II. PROCEDURE

The flow chart used to develop the electronic textbook for chemical experiment is shown in Figure 1. The chemical reaction was selected based on its importance in fundamental chemistry. To exhibit phenomena (left side), the experimental condition was optimized for college level small-scale chemistry-experiment.

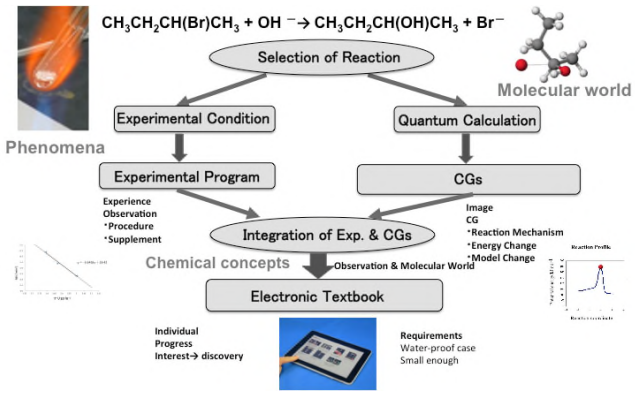

Figure 1. Flowchart of Developing Tablet for Chemistry-experiment

To provide the image of the molecular world (right side), CG images such as realistic shape of molecules and the CG movies of reaction mechanisms were made, based on the quantum chemistry calculation [5], [6]. A movie of the

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reaction path was produced by the software DIRECTOR (ver. 8.5.1J, Macromedia, Inc.) following the display of the bond order of the structures of the reactants in each reaction stage, which was drawn by SCIGRESS (Fujitsu). The obtained CG was combined with the reaction profile in the same reaction stage. It was confirmed that the drawn CGs of the molecular models of reactants moves smoothly. A ball, which indicates progress of the reaction, was arranged on the reaction profile and simultaneous movements of the ball and the reactants were confirmed. The created movie file was converted to the Quick Time movie for iPad by the Quick Time PRO (ver. 7.66, Apple, Inc.). After the combination of the experimental section and the CG section, the electronic textbook was produced with iBooks Author (ver. 2.1.1, Apple, Inc.) and was saved to tablet (iPad, Apple, Inc.) by using iTunes (ver. 11.2.1, Apple, Inc.). In order to use the electronic textbook on the lab bench, it needed to be covered with a waterproof, Zip-lock type, case.

III. PRESENTATION ON TABLET

In the experimental section, enlargeable-photos and flow charts were used for easier understanding of the procedure, in addition to regular text-base description. Supporting information, such as properties of reactants, was also included. The electronic textbook could acts as an individual electronic tutor.

The CG movie, shown in Figure 2, can simultaneously demonstrates the nature of the reaction, such as structural changes by the space-filling model and by the ball-and-stick model, in addition to providing an image of energy change by the reaction profile. Students are able to rotate the molecule freely and observe molecular geometry by touching 3D-CG on the right side of the text. Students are expected to obtain the image of an "umbrella reverse" like motion in the Walden's inversion while they are watching the actual reaction progress. This way, the experimental observable level and the molecular world could be integrated.

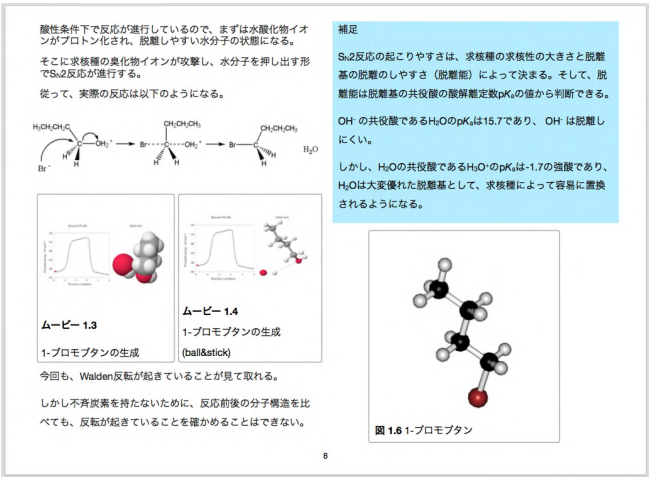

Figure 2. CG movies and 3D-CG of 1-bromobutane formation

IV. CONCLUSION

We developed computer graphics teaching material for university students, concerning chemical reactions with drastic change in the structure of reactants. The following chemical reaction was an example of Walden's inversion: hydroxylation of methyl chloride, formation of 2-butyl alcohol and 1-butyl bromide. The CG could demonstrate the drastic change of the structure and the reaction profile can provide an image of the energy change during the reaction. The textbook could display the picture of apparatus and a flow-chart of the experiment in addition to CG. From the preliminary study, students were able to obtain images of structural changes and conduct experiments smoothly and safely with the electronic textbook inserted in the Ziploc type plastic bag. The developed electronic textbook on the tablet could be used to integrate the experimental observable level and the molecular world.

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