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Development and Practice of Electronic Lab Book for College Chemistry Experiment - S_N1 and S_N2 Reactions

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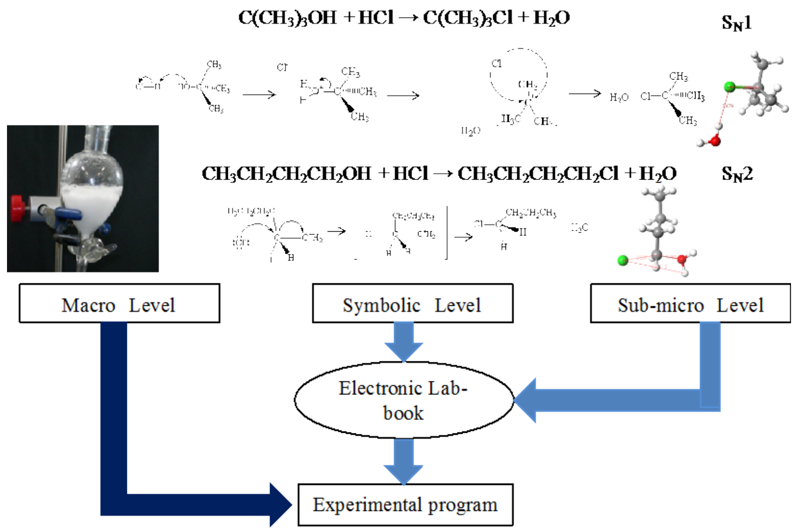
Abstract: We developed a computer graphics (CG) teaching material (TM) for university students, concerning reactions involving drastic changes in the structure of the reactants in the following chlorination, for example S_N1: formation of tert-butyl chloride from *tert*-butanol and S_N2: formation of 1-chlorobutane from 1-butanol. The CG-TM could clearly demonstrate the changes in the structures during the reaction by the ball-and-stick model, in addition to the image of the energy change in terms of the reaction profile. An electronic lab-book for chemical experiments in the students' laboratory at the university was produced, aiming at the integration of observable-level experiments, symbolic chemical equations, and the molecular world. The lab-book displays pictures of apparatus, flow-chart of experimental procedures, and reaction mechanisms with the CG-TM. A preliminary study on the effectiveness of the CG-TM suggested that students were able to obtain images of S_N1 and S_N2 reactions.

Keywords: CG, Visualization, Chemical reaction, Electronic textbook, Chemical experiment

1. Introduction

We are attempting to produce a computer graphics teaching material (CG-TM) based on quantum chemistry calculations, which provides accurate and realizable images of the nature of a reaction (Ikuo, 2006 and 2009). It has been reported that molecular-level animations combined with video clips of macroscopic phenomena enable students to predict the outcome of a chemical reaction better (Velazquez-Marcano, 2004). Many electronic textbooks of chemistry are available, but most of them are very similar to hard copies and very few are related to chemical experiments (Morvant, 2013). Moreover, a combination of the CG movie of a reaction and an experiment is not available. If the CG can be combined with a lab-book of chemical experiments, students can observe the reaction from three levels of thinking (Gilbert, 2009 and Tasker, 2010): molecular-level CG, which enables students to obtain a realistic image of a symbolic-level chemical equation, and the phenomenon of an actual reaction. Our ultimate goal is to produce an electronic lab-book for chemical experiments, which integrates these three levels of thinking.

Nucleophilic substitution (S_N) reactions, in which a nucleophile displaces another group or atom from a compound, are among the basic reactions in organic chemistry. Therefore, the S_N reaction is often adopted in TM on the university curriculum, including appropriate schemes that aim to show drastic changes in the molecular structure (McMurry, 2001). TMs or schemes that enable students to provide realizable images of the nature of a reaction need to be developed. We have reported that an electronic lab-book with CG-TM is a promising means to provide images of the Walden inversion during the S_N2 reaction (Ikuo, 2012). This paper describes our work on the CG visualization of the chlorination of both *tert*-butanol and 1-butanol as an example of S_N1 and S_N2 reactions, in order to provide realistic images of the mechanisms underlying both types of nucleophilic substitution reactions (Scheme 1). The CGs showing the molecular world and experimental procedures for the students' laboratory at the university are combined in the electronic lab-book in order to integrate the observable-level experiment, symbolic-level chemical formula, and the molecular world for the nucleophilic substitution reaction. A preliminary study on the effectiveness of the CG-TM is also reported.



Scheme 1. Development of Electronic Lab-book.

2. Development

In STEP1, the S_N1 reaction mechanism is introduced first; then, a learner is expected to grasp a three-dimensional rearrangement image of the reactant molecules during the reaction by watching the CG and CG movie along with the chemical equation and scheme. Subsequently, the stereochemistry is studied using CG. Finally, the reactivity is studied. The S_N2 reaction is studied in a similar manner. This step may take approximately 20 min, which can be assigned as homework. In STEP2, the actual S_N1 and S_N2 reactions are introduced. Chlorination of both *tert*-butanol for S_N1 and 1-butanol for S_N2 is conducted. The infrared spectral data of the products and reactants are compared. This step may take approximately 2.5 h for each reaction. In STEP3, the learner is expected to integrate his/her knowledge about the S_N1 and S_N2 reactions by participating in a quiz.

The semi-empirical molecular orbital calculation software MOPAC with PM5 Hamiltonian (Stewart, 1989) in the SCIGRESS (ver. 6.01, FUJITSU, Inc.) was used for determination of structures of reactants to products on the reaction path. A movie file was produced by the SCIGRESS and was converted to the image-sequence file by the Quick Time PRO (ver. 7.66, Apple, Inc.) and was compiled with Director (ver. 12.0, Adobe, Inc.). An electronic textbook was produced with iBooks Author (ver. 2.5, Apple, Inc.) and was saved to the tablet (iPad Air2, Apple, Inc.) by using iTunes (ver. 12.5, Apple, Inc.). The CG-TM could clearly demonstrate the changes in the structures during the reaction by the ball-and-stick model, in addition to the image of the energy change in terms of the reaction profile. An electronic lab-book for chemical experiments in the students' laboratory at the university was produced, aiming at the integration of observable-level experiments, symbolic chemical equations, and the molecular world. The lab-book displays pictures of apparatus, flow-chart of experimental procedures, and reaction mechanisms with the CG-TM (Ikuo, 2017).

3. Practicing the Use of the Electronic Lab-book

Five first-year students, four second-year students, and four third-year students in chemistry department of the teachers' training course at Tokyo Gakugei University, who took or were going to do basic organic chemistry in the first year, were asked to practice STEP1 (grasp the image of S_N1 and S_N2 reactions) and STEP3 (quiz part of the electronic lab-book). First, the usage of the tablet was explained, and then, a pre-test was conducted. After the pre-test, tablets were distributed to each student, and the students were asked to study STEP 1 and try to answer the questions in STEP 3. Finally, a post-test was conducted. Students were confirmed to concentrate on the subject, as they studied STEP 1 in detail and attempted to answer the questions in STEP 3.

Table 1 presents the results of the questionnaire. The average score of correct answers were 2 out of 6 in the pre-test, except second year students who just finished organic chemistry class, and they were increased to 5.2 or better in the post-test. After using the electronic lab-book, students' knowledge in terms of "reactivity," "attacking direction," and "energy change" in the S_N1 and S_N2 reactions was improved. The students added their comments in the free description section of the questionnaire, for example, "After using iPad, image of the reaction became certain" and "the movie helped understanding the reaction mechanism." These comments suggested that the electronic lab-book could provide an image of the S_N1 and S_N2 reactions.

Although a more detailed study needs to be carried out on the effectiveness of the electronic lab-book, we can state that the students could obtain an image of the S_N1 and S_N2 reactions.

Table 1: Effect of Electronic Lab-book on Number of Correct Answers for Different Classes

#	Question	Before Org. Chem.*		After Org. Chem.**		2 years after**	
		Pre	Post	Pre	Post	Pre	Post
1	Reactivity in S_N2	2	5	4	4	1	3
2	Reactivity in S_N1	2	4	4	4	1	4
3	Attack direct. & product in S_N1	1	5	1	4	1	4
4	Attack direct. & product in S_N2	2	5	4	4	3	3
5	Stereo-chem. in S_N1 & S_N2	2	4	4	4	2	3
6	React. energy in S_N1 & S_N2	1	3	3	3	0	4
	Average score***	2.00	5.20	5.00	5.75	2.00	5.25

*: number of students = 5; **: number of students = 4; ***: full-marks=6, one point for each question

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