Development of teaching material in tablet PC based on computer graphics by quantum chemistry calculation - Walden's inversion

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Abstract: We developed computer graphics (CG) teaching material (TM) for university student, concerned about reaction with drastic change of the structure of reactants in following reaction as a model of Walden's inversion; $OH^- + CH_3Cl \rightarrow CH_3OH + Cl^-$. The CG-TM could demonstrate the nature of the reaction by space filling model, ball-and-stick model, and the reaction profile that can provide image of energy change during the reaction. The CG-TM enabled to load with note PC, tablet PC, and smart phone. Practice to the first year or the second year student of Tokyo Gakugei University was conducted. Surveys revealed that the CG-TM in tablet PC was sufficiently effective to provide information about the nature of the Walden's inversion.

Keywords: Teaching material, CG, Visualization, Tablet computer, Quantum chemistry calculation, Walden's inversion, Structure change, Space filling model

Introduction

Visualization of computer graphics (CG) gives us great help to realize not only images of molecular properties but also those of molecular behavior on dynamical reaction mechanism. It is our aim to produce CG teaching material (CG-TM), which provides realizable images of the nature of chemical reaction [1]. Walden's inversion is one of typical reactions in organic chemistry, and the reaction is often adopted in TM on the curriculum of the university, including some appropriate schemes [2]. The schemes should be developed for student to acquire more realizable images of the nature of the reaction. We developed CG-TM for university student, concerned about reaction with drastic change of the structure of reactants in the reaction (Eq. 1) as a model of Walden's inversion.

$$OH^- + CH_3Cl \rightarrow CH_3OH + Cl^- \qquad \text{(Eq. 1)}$$

Production of CG-TM by quantum chemistry calculation and practice of the CG-TM in tablet computer, which is more effective to provide image than that with PC and the projector [3], to the university student are reported.

1. Procedure

1.1 Quantum chemical calculation

The semi-empirical molecular orbital calculation software MOPAC with PM5 Hamiltonians [4] in CAChe Work System for Windows (ver. 6.01, FUJITSU, Inc.) was used to find the transition state and the reaction path of chemical reactions. The structure of the reactants on the transition state was searched by use of the optimized map with the PM5 energies (One Label) in MOPAC with the model described in above. 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 for vibration analysis. If the peak was observed, Intrinsic Reaction Coordinate (IRC) [5] calculation was done and the reaction path was confirmed.

1.2 Production of CG teaching material

A movie of the reaction path was produced by the software DIRECTOR (ver. 8.5J, 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. 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.) and iPhone 4 (Apple, Inc.), by using the iTunes (Apple, Inc.).

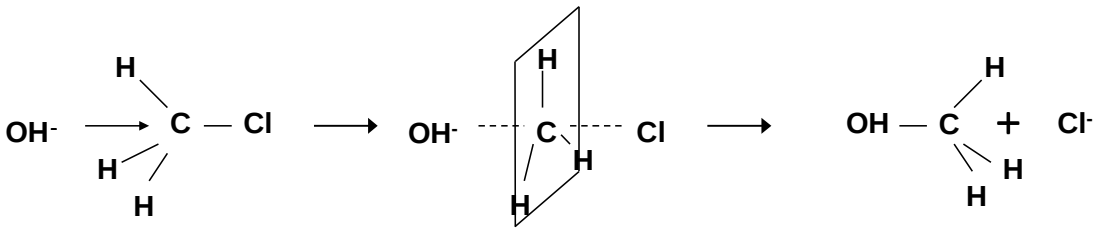
1.3 Practice of teaching material

Teaching material was practiced on three classes, the first year student of teacher training course for elementary school and the second year student of natural environmental science course, of “Chemistry laboratory” in the fall semester of the 2010 fiscal year at Tokyo Gakugei University. Total numbers of students were 103. All practice was carried out by one instructor and one teaching assistant. Teaching material used for the trial was the CG movie of ball –and-stick model shown by the tablet PC. Procedure of the practice is described as follows. Preliminary survey, which consisted questions to ask them to draw image of Walden’s inversion from formula and questions about information of students, were conducted. Then, usage of the tablet was explained by instructor with projection of the CG movie. After the explanation, 9 tablet PCs were distributed to students and asked them to watch CG movie in the tablet as shown in the figure 1. Students started to touch it and watched the movie over and over enthusiastically. One tablet PC was shared by two to four students depends on size of class. Time duration for usage of the tablet PC was about three minutes for each student. During this time period students were quiet which suggests that they were concentrated on the subject. After about 10 minutes, students were asked to start answer the posteriori survey that consisted question to ask them to draw image of Walden’s inversion from the movie. Some students were still watching the movie even when they were answering the questionnaire.

Figure 1 Practice of teaching material

2. Results and discussion

2.1 CG teaching material



Scheme 1 Images of Walden's inversion

The S_N2 reaction of chloromethane and hydroxide [2] is shown in the scheme 1. Carbon atom at center to which halogen attaches is attacked by the nucleophile, hydroxide, from a position away by 180 degrees and methyl alcohol forms. Therefore, the transition state was searched from the reactants where the bond angle of O-C-Cl was adjusted to 180 °. A single absorption peak in the negative region was found at -399.46 cm^{-1} from the vibrational analysis. This result indicates vibrational mode due to the decrease of potential energy for the direction of only one path via a true transition state at the saddle point.

The reaction path from the reactants to the products via the transition state was searched by the intrinsic reaction coordinate (IRC) calculation [5] in MOPAC. The inter-atomic distances, *d*, and the heat of formation obtained by the calculation are listed in the scheme 2 and in the table. These values were in good agreement with the literature values [6, 7]. Therefore, it was confirmed that the reaction path and the molecular configurations obtained by the calculation were appropriate.

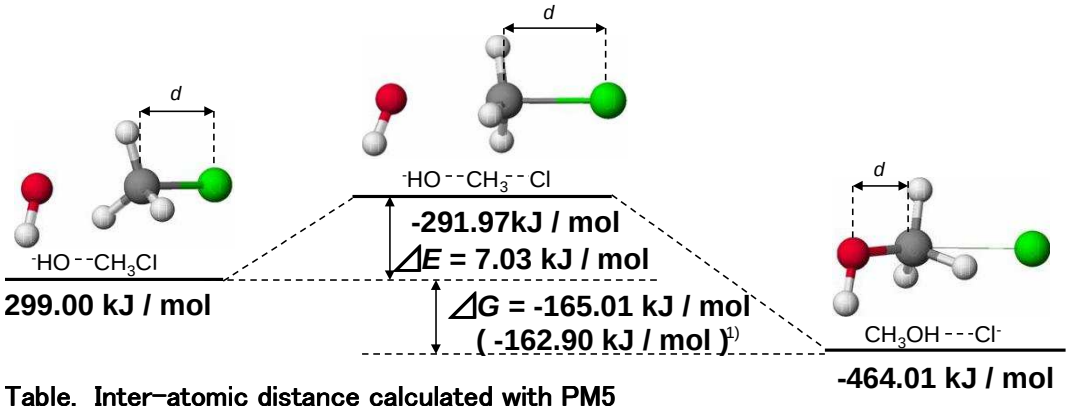


Table. Inter-atomic distance calculated with PM5

Sample	*d* / Å		
	Calculation	Experimental	Subtraction
$^-HO\cdots CH_3Cl$	1.87	1.78 [2)]	0.09
$^-HO\cdots CH_3Cl\cdots Cl^-$	2.16		
$CH_3OH\cdots Cl^-$	1.41	1.43 [3)]	-0.02

Scheme 2 The structures of the initial state, the transition state and the final state of formation methyl alcohol and energy

The literature values are indicated in the parentheses.

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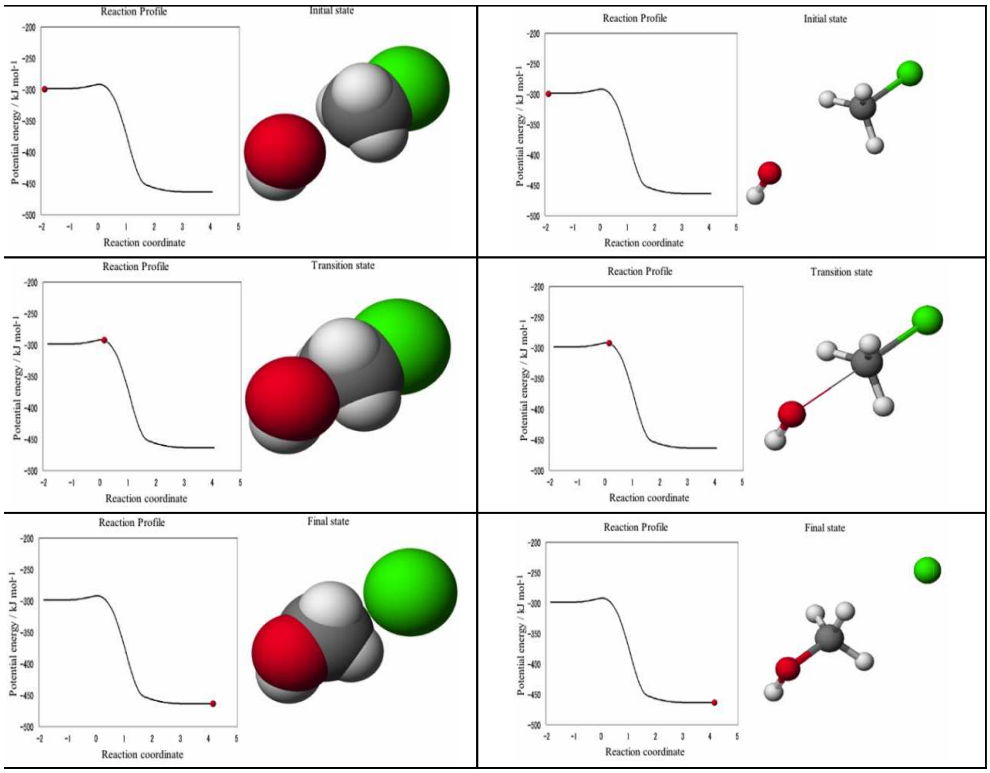
2.2 Teaching material

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

Figure 2 Selected picture of CG movies
Reaction profile and image of reactants in space filling and ball-and-stick model



2.3 Evaluation

The result of the questionnaires was summarized. 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 Walden's inversion from the CG teaching material.

3. Conclusion

In this work, the change in the molecular configuration in Walden's inversion made visible from the quantum chemistry calculation. The CG teaching material enabled to load with note PC, tablet PC, and smart phone. Surveys revealed that the teaching material in tablet PC was sufficiently effective to provide information about the nature of the Walden's inversion.

Acknowledgements

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