T. Hirashima et al. (Eds.) (2011). Proceedings of the 19th International Conference on Computers in Education. Chiang Mai, Thailand: Asia-Pacific Society for Computers in Education

Development of teaching material in tablet computer based on computer graphics by quantum chemistry calculation

– Reaction of $I + H_2 \rightarrow HI + H$ –

Akira IKUO[a]*, Hiroshi NAGASHIMA[a], Yusuke YOSHINAGA[a] & Haruo OGAWA[a]

[a] *Department of Chemistry, Tokyo Gakugei University, Tokyo 184-8501, Japan.*
*ikuo@u-gakugei.ac.jp

Abstract: We developed computer graphics teaching material in tablet computer, which shows rearrangement of diatomic molecule and one atom by collision. The teaching material provides information concerning changes of potential energy and realistic image of intermediate in $I + H_2 \rightarrow HI + H$, which leads to better understanding of reaction profile.

Keywords: Teaching material, CG, Visualization, Tablet computer, Quantum chemistry calculation, HI formation, Potential Energy change, Structure change.

Introduction

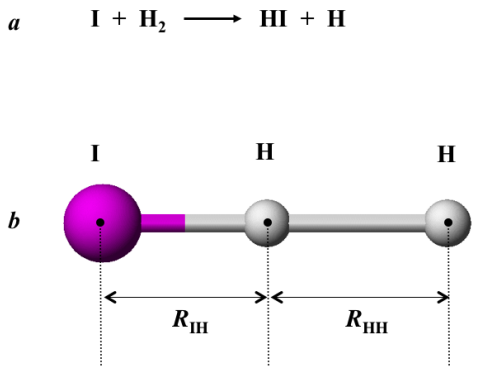
Generally, reaction profile is used to represent relationship between potential energies (PE) and reaction coordinate. The profile is often used in high school chemistry textbooks [1a-e]. It is sometimes difficult for student to realize the meaning of reaction coordinate. Visualization of computer graphics (CG) gives us great help to realize not only images of molecules but also images for dynamical reaction mechanism. Visualization of PE surface in three dimension (3-D) could clearly provide images of reaction coordinate from the standpoint of subject on energy. A diagram of PE in two dimension (2-D) is often used, and limited number of analogues in 3-D is used in physical chemistry textbook of university [2a,b]. It is our aim to produce teaching materials, which provide realizable images of chemical reactions. Recently, CG teaching material of esterification of acetic acid and ethyl alcohol based on quantum chemistry calculations has been reported [3]. The teaching material could demonstrate the reaction profile and structural change of the molecules with ball-and–stick model on screen.

The reaction of "$I + H_2 \rightarrow HI + H$" is often used for explanation of reaction rate and chemical equilibrium in "Chemistry II" of Japanese high school [1d], but the reaction path and the change of PE during reaction are explained by ambiguous expression based on old model [4]. Mechanism of the reaction has been reported that HI formation progressed as following elementary reactions [5]; $I_2 \rightarrow 2I$ (Eq. 1), $I + H_2 \rightarrow HI + H$ (Eq. 2), $H + I \rightarrow HI$ (Eq. 3)

We developed CG teaching material in tablet computer, which shows rearrangement of diatomic molecule and one atom by collision. The teaching material provides information concerning changes of PE and realistic image of intermediate in the Eq. 2, which leads to better understanding of reaction profile.

1. Procedure

The reaction images of an attack of iodine atom (I) to hydrogen molecule (H_2) in the formula (*a*) and in the ball-and-stick model (*b*), in which diameter of the stick reflects calculated bond order, are shown in scheme 1. Bond angle of I-H-H was set to 180 ° and inter-atomic distances of I-H (R_{IH}) and H-H (R_{HH}) were changed. PE and structures of intermediates of I-H-H on the way of the reaction were calculated by MOPAC with PM3 Hamiltonians [6a-c] as described previously [7].CG movie file was produced by the Flash CS4 software (Adobe, Inc.). The movie file was converted by the Quick Time PRO (ver. 7.66, Apple, Inc.) and was saved on iPad (16GB, IOS4.3.3, Apple, Inc.) by using the iTunes (ver. 10.22, Apple, Inc.).



Scheme 1. Reaction of a) "I + H_2" and b) image of inter-atomic distance

2. Results and discussion

Figure 1 shows CG teaching material in tablet computer. Upper right part of the CG shows PE change in 3-D and lower right part in 2-D. In this way learner can compare two types of presentation easily. In 2-D presentation, inter-atomic distance of I-H (R_{IH}) is drawn as a horizontal axis and that of H-H (R_{HH}) is as a vertical axis; therefore, learner can see relationship between changes in inter-atomic distances of I-H, H-H, and change of PE in color change. Upper right part of the CG clearly shows these changes of PEs with display on PE surface in 3-D, which offers a bird-eye view of the reaction profile. The most probable pathway 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 right part of CG is able to provide images of energy change and reaction path.

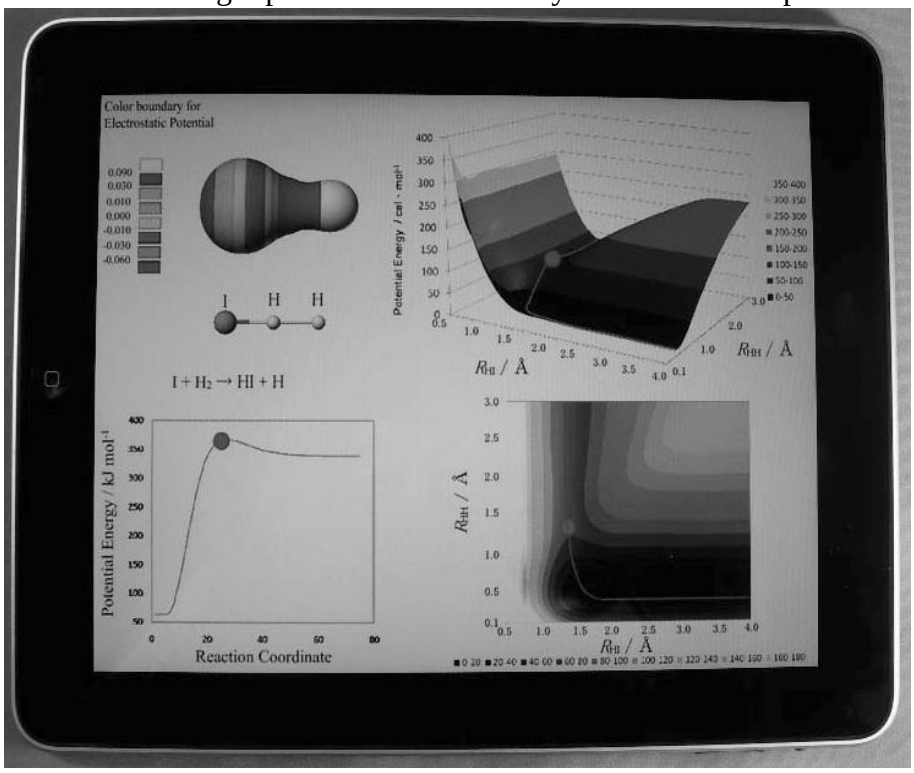


Figure 1. CG teaching material in tablet computer

Electrostatic potential on electron density (EPED) model and ball-and-stick model of the intermediate, I-H-H, and the reaction profile were shown in the left part for easier recognition of those three. The electrostatic potential [8] was calculated based on the coordinates of atoms from the intrinsic reaction coordinate (IRC) calculation 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 of the CG. Distribution of the electrostatic potential among the

intermediate can be seen by the colors. The model by EPED provides information about electrostatic distribution of the intermediate with realistic shape on the way of the reaction. Lower left part of the CG shows the reaction profile, the most probable pathway of chemical reaction according to the IRC theory [9], demonstrates the degree of the reaction progress by the ball indicating PE *vs.* reaction coordinate. The left part of CG is able to provide information about characteristics of intermediate of molecule in a certain state on the progress of reaction.

This CG teaching material is able to provide information about energy change, reaction path, and characteristics of intermediate of molecule in a certain state on the progress of reaction simultaneously. In this synclonized display of CGs, lerner can see relationship between the reaction path in 3-D and the reaction profile in 2-D. When the CG in the touch-panel is touched by learner, the Quick Time control bar appears and the ball on the profile can be moved by learner's choice. This manual controll feature provides "Hands-on" feeling to learner.

3. Closing

The CG teaching material could provide not only images of energy change during reaction but also images of reaction path of chemical reaction. The teaching material could be used in the high school, of course in the university, as a supplement to the figure of reaction profile often found in the subject of "structure and the chemical equilibrium of the material" in the high school chemistry textbook [2a-e] edited accodingly the Japanese course of study [10] and also in the university textbook [1a,b]. The teaching material in the tablet computer is so handy that it could be used in both regular class and laboratory.

Acknowledgements

This work was supported by JSPS Grant-in-Aid for Scientific Research (C) (22500803).

References

[1] a: Daiichigakusyusya (2004). *Chemistry II* (in Japanese); b: Jikkyosyuppan (2004). *Chemistry II* (in Japanese); c: Keirinkan (2003). *Chemistry II* (in Japanese); d: Sanseido (2004). *Chemistry II* (in Japanese); e: Tokyosyoseki (2004). *Chemistry II* (in Japanese).

[2] a: Atkins, P., & Paula, Y. (2002). *ATKINS Physical Chemistry* 7th. Ed., 966-969, OXFORD UNIVERSITY PRESS; b: Moor, W. J. (1982). *PHYSICAL CHEMISTRY*, 4th. Ed., pp. 382-387, Tokyo Kagakudojin (in Japanese).

[3] Ikuo, A., Ikarashi, Y., Shishido, T., & Ogawa, H. (2006). USER-FRIENDLY CG VISUALIZATION WITH ANIMATION OF CHEMICAL REACTION: ESTERIFICATION OF ACETIC ACID AND ETHYL ALCOHOL AND SURVEY OF TEXTBOOKS OF HIGH SCHOOL CHEMISTRY, *Journal of Science Education in Japan*, **30** (4), 210-215.

[4] Bodenstein, M. (1893). *Ber*., **26**, 2603.

[5] Sullivan, J. H. (1967). Mechanism of the "Bimolecular" Hydogen-Iodine Reaction, *J. Chem. Phys*., **46** (1), 73-78.

[6] a: Stewart, J. J. P. (1989). *J Comp. Chem*., **10**, 209–220; b: Stewart, J. J. P. (1989). *J. Comp. Chem*., **10**, 221–264.; c: Stewart, J. J. P. (1991). J. Comp. Chem., **12**, 320–341.

[7] Ikuo A., Nagashima H., Yoshinaga Y., & Ogawa H. (2009). Calculation of potential energy in the reaction of "I + H2 → HI + H", and its visualization, *The Chemical Education Journal (CEJ)*, Registration #13-2.

[8] Kahn, S. D., Pau, C. F., Overman, L. E., & Hehre, W. J. (1986). Modeling chemical reactivity. 1. Regioselectivity of Diels-Alder cycloadditions of electron-rich dienes with electron-deficient dienophiles, *J. Am. Chem. Soc*., **108**, 7381-7396.

[9] Fukui, K. (1970). *J. Phys. Chem*., **74**, 4161-4163.

[10] MEXT (1999). *Japanese course of study (high school)*.