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Profile of Students' Comprehension of 3D Molecule Representation and Its Interconversion on Chirality

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Abstract. This study aims at describing (1) students' level comprehension; (2) factors causing difficulties to 3D comprehend molecule representation and its interconversion on chirality. Data was collected using multiple-choice test consisting of eight questions. The participants were required to give answers along with their reasoning. The test was developed based on the indicators of concept comprehension. The study was conducted to 161 college students enrolled in stereochemistry topic in the odd semester (2014/2015) from two LPTK (teacher training institutes) in Bandar Lampung and Gorontalo, and one public university in Bandung. The result indicates that college students' level of comprehension towards 3D molecule representations and its inter-conversion was 5% on high level, 22 % on the moderate level, and 73 % on the low level. The dominant factors identified as the cause of difficulties to comprehend 3D molecule representation and its interconversion were (i) the lack of spatial awareness, (ii) violation of absolute configuration determination rules, (iii) imprecise placement of observers, (iv) the lack of rotation operation, and (v) the lack of understanding of correlation between the representations. This study recommends that learning show more rigorous spatial awareness training tasks accompanied using dynamic visualization media of molecules associated. Also students learned using static molecular models can help them overcome their difficulties encountered.

INTRODUCTION

Molecule **'chirality'** refers to molecules unable to be superposed to their mirror images, similar to our right and lefts hands (in Greek, *cheir;* hands*)*. On the contrary, the super-possable molecules are considered as **achiral.** Chiral molecules are asymmetric.[1,2] In the study of stereochemistry, molecule chirality is an important subtopic. Therefore, students' deepen comprehension on the chirality concept were expected to be able to explain numerous natural phenomena. For instance, *"the building blocks of life*", *i.e.*α-amino acid, nucleotide, and monosaccharide, are chiral, and exists as a pure enantiomer. In addition, every substance produced or modified by human, such as medicine, will ultimately interact with chiral environment. This problem draws a serious attention from experts in the field of bioorganic chemistry and pharmacy chemistry.[3]

There are a number of techniques to represent 3D chiral molecules in stereochemistry lesson. Representation was used to provide varied specific information based on official rules. Thus, the ability to interpret the connection of one representation to another was considered as a vital part of conceptual or comprehension model.[4] Among varieties of methods to represent the position of atoms/molecule clusters in 3D area as Dash-Wedge representation, ball-and-stick, Newman projection, and Fischer projection.[5]

Some writers reported that students have difficulties in comprehending symbolic representation of three-dimensional structure of chemical molecules.[6] Some other researchers also conveyed that the use of 2D symbolic representation to visualize 3D structure of molecules was a complex cognitive task and demands for considerable skills to interpret the connection of both.[7,8] Therefore, stereochemistry was considered as a problematic and confusing field of study for students.[9] Indeed, when studying about stereochemistry, students expected be able to

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visualize the three-dimensional representation of molecules in two dimensions as well as perform a variety of 'space task' requiring representations, rotation, and inversions of 3D objects as they are represented in 2D.[10,11]

So far, there have been several reports that examine the dominant factors that contribute to the difficulty in understanding the 3D representations of molecules and also its interconversion, but there is no discussion in the report which includes an analyzing students' logical steps as a problem solving strategy when converting among the representations [4,12,13]. In this article, in addition to revealing the dominant factors causing difficulties when student comprehend the molecular representation of 3D and its interconversion on the topic chirality, also presents of logical thinking in problem solving. This is believed to be the author of a novelty in the study.

Logical thoughts to solve problems related to representation and its inter-conversion, were expected to contribute significantly on points to be highlighted and enhanced in dealing with the implementation strategy and utilization of appropriate media to develop students' ways of thinking in order to comprehend 3D representation of molecules and its interconversion. In this research, questions were organized based on conceptual indicators discussed in the subtopic of molecule chirality, including enantiomer, determination of absolute configuration based on R/S notation proposed by Chan-Ingold-Prelog, Fischer Projection, and interconversion among representations.

METHOD

This research was conducted under descriptive quantitative analysis method. The subject of the research was 161 students from three institutes; two LPTKs located in Bandar Lampung and Gorontalo, and one non-LPTK Institute in Bandung. The students acquired a lesson on Stereochemistry in the odd semester of the year 2014/2015.Technique of data collection implemented in this study was a test. The selection of this technique was intended to uncover factors contributing of difficulties in comprehending 3D representation of molecules and its inter-conversion within a study on chirality. Test instrument was designed as multiple choice questions with rationality, organized according to conceptual mastery indicators on molecule chirality. There are eight test items comprising four items, numbered 1,2,3, and 8, to identify comprehension on 3D representation of molecules, and the other 4 items, numbered 4,5,6, dan 7, to recognize students' comprehension on representation interconversion. The highest score for each item is 3; 1 score for selecting correct option, and maximum 2 scores for reasons given. In total, the maximum score is 24. Students are considered to perform excellent comprehension with score ≥ 17, moderate comprehension with score lower than 17 but higher or equal to 9; and low comprehension with score ≤ 8. The formula to calculate the percentage of level of comprehension category is by the following formula: $v_{ave} = \left(s_i / m \right) \times 100\%$, where v_{ave}, s_i, and m are the percentage of level of comprehension category, the number of students who obtain score in each category level, and the total number of students, respectively.

RESULTS AND DISCUSSION

Profile of Student's Comprehension on the Representation of 3D Molecules and Its Inter-conversion on Chirality

In this study, the categorization was based on the level of students' comprehension of the obtained magnitude score. The study showed that of 161 students, there were as many as 5% of students categorized as having a high level of comprehension, 22% had a moderate level of comprehension category; and there were as much as 73%, are categorized as low level or "having difficulty" in comprehension the 3D representation and its interconversion. The result of analysis on test record classification of student's comprehension on molecule representation, and its inter-conversion inferred following profile of students' comprehension, as presented in **Figure 1**.

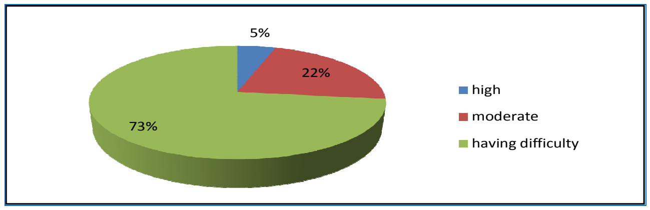

FIGURE 1. Profile of students' comprehension of 3D molecules and its inter-conversion chirality

The average number of students who correctly answered to the four question in the first category to measure comprehension the molecular 3D representation was as much as 41.4%, and the average number of students who answered correctly on the four questions in the second category to measure comprehension of the inter-conversion of representation there as much as 24.8%, is presented in **Figure 2b**.

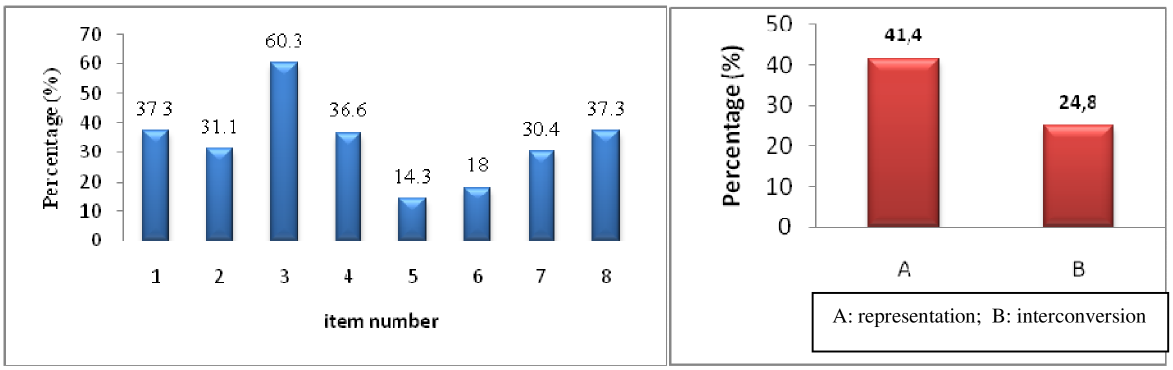

FIGURE 2.(a) Profile of the number of correct answers for each multiple choice questions; (b) Profile of the number of correct answers for questions on representation and inter-conversion.

Factual data presented above suggest that most students had difficulties in answering each question related to their comprehension on 3D representation of molecules also its interconversion. However, in general, it can be indicated that students were more competent to solve questions on the representation concept than those on inter-conversion from one type of representation to another. This condition can be closely related to the complexity and proficiency student's ways of thinking.[10] As dealing with 3D representation of molecules, one will imagine a structure of atoms/clusters within a space according to prevailing notation or symbols as rules and media of interpretation of symbols into real situation.[7] For instance, a molecule with one chiral carbon atom is represented with Dash-Wedge representation, so that someone may imagine the orientation of clusters/atoms adjacent to bond notation and symbols portrayed. It shows which clusters/atoms located in the structure, away from the observer, and toward the observer. Likewise, even though Fischer Projection is portrayed in the 2D image, as it is used for 3D representation of a molecule, someone is demanded to imagine the structure of atoms in a tetrahedral space around C chiral atoms, corresponding to their positions on vertical or horizontal lines. In this research, such as tasks were also considered as problematic for almost 60% of the students. This condition is in agreement with what was reported by some other researchers asserting such a difficulties.[6,11] The level of complexity of thinking process certainly increased along with tasks related to modification from one type of representation to another.

To cope with tasks for modifying 3D representation of molecules, someone has to dig his long-term memory about symbols and rules for each representation and determine the relation among the representations. It is the combination of the knowledge of those symbols and relations that will result in fresh skills necessary as modifying one representation to another, and moreover, from 2D representation, such as Fischer projection, to 3D representation and vice versa. This perception was also reflected in some previous studies suggesting that 3D visualization of molecules using 2D symbolic representation is an exceedingly complex task and requires different types of proficiency to interpret it. [7,8]

By reviewing the result of study presented in Picture 2, based on the number of students giving the answers, it can be perceived that question number 2 about 3D representation of a molecule had the highest level of difficulty. Similar condition occurred among questions about interconversion from one representation to another. Then, why was question number 5 considered as a 'very complex' one? What factors resulted in such difficulties?

Factors contributing of difficulties in comprehending 3D representation and its inter-conversion

The most difficult test item about representation, question No. 2, was presented in **Figure 3**. Problems developed to measure students' comprehension of the 3D representations of molecules, related to enantiomer concepts was labeled with one chiral center.

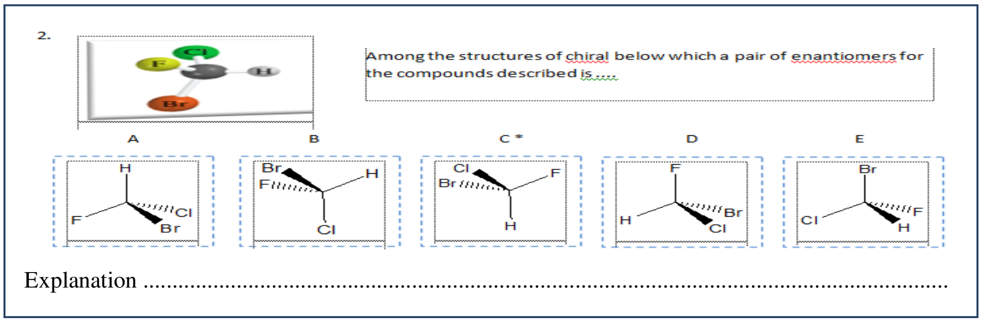

FIGURE 3. Tes item no 2

Cognitive stages to answer test item number 2 are (i) carefully observing 3D images of molecules in test items represented with ball-stick notation. At this point, a student could consider himself as an observer, imagining spatial orientation of atoms around carbon chiral atom. Someone's mind should properly construct a tetrahedral space with C atom as the center and atoms directing to the corners. Based on the structure given, there should be an image that atom H and Br are located in the same structure; F is toward the observer, but Cl is away from the observer;(ii) transforming the orientation of those atom's structure into the representation of dimensional structure based on notation instruction (iii) identifying the absolute configuration based on CIP rules; the absolute configuration analyzed is R, and (iv) verifying the absolute configuration of the five options; considering a pair of enantiomers usually have contradictory absolute configuration, one may determine that the best option was C.

Figure 4a was an example of students' reasoning of choice E option. This student showed imprecise positioning of representation of the image on his or her reason. These resulted in imprecision translating it into notation conventions as agreed. The analysis showed that the inability to capture and interpret spatial information in question experienced by 68.9% of students. The study supports the results of research which states that the trouble to study the stereochemistry comes from a lack of mastery technique to place the observer, and lack of precision in the application of different representation conventions.[4]

Figure 4b was an example of the reason for choosing option C. Although choosing the appropriate option, based on the analysis, there were as much as 78.3% supplied partial correct response reasons. Reason indicates that they had the accuracy of positioning as an observer, able to capture the imagination of the spatial structure of the molecule, but have not could to represent another structure connected as enantiomers and marks the absolute configuration. The finding was in line with the statement of researchers that studied the representation of 3D visualization of molecules is a complex task and requires a variety of skills to interpret this relationship.[9]

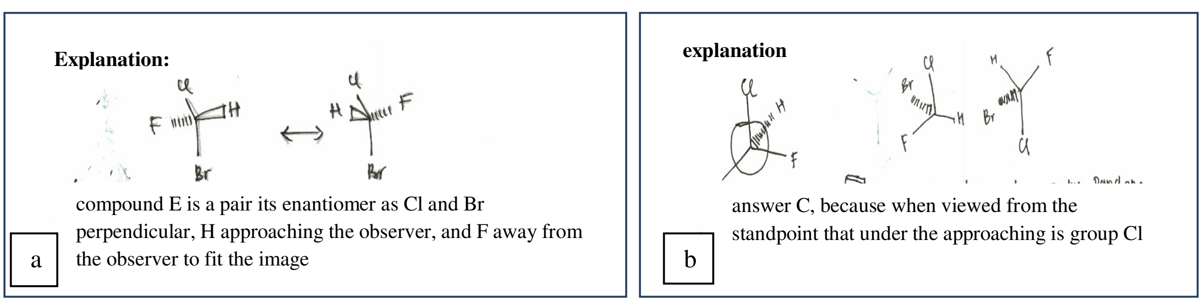

FIGURE 4.(a) An example of student's rationality for correct answer ; and (b) an example of student's rationality indicating partial entity, but accurate option, for item number 2.

The results the study in the interconversion representations **(Figure 2b)** showed there were 75.2% of students had difficulty of interconversion. Problem number 5 was intended to measure students' comprehension of chiral molecules change the representation of the formula dimensional projection to Fischer and the vice versa. **Figure 5a** presents the test items, while profile of the percentage of multiple choices answers options presented in **Figure 5b**.

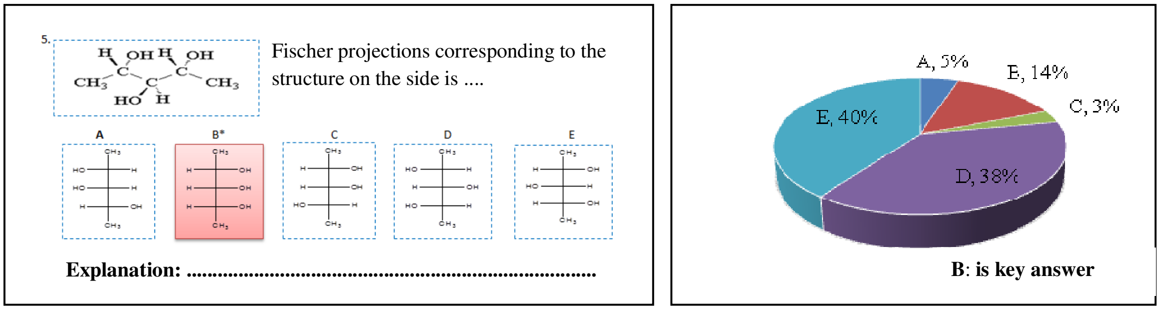

FIGURE 5.(a) Test Item Number 5; (b) Profile of the Number of Students' Answers on Multiple Choice Questions

The cognitive stages to solve inter-conversion problems from Dash-Wedge representation in test item number 5 are (i) finding the main carbon framework and numbering it; (ii) setting observer orientation based on Fischer projection rules, so that C number 1 can be on the top (away from observer), (iii) (a) the position of OH and H clusters in C number 3 was still away from the observer, so that sigma bond connecting C number 3 to C number 2 and 4 had to be rotated by 180^o, (b) the observer checked Newman projection through the center of projection of C_1-C_2 because the position of OH/OH and H/H clusters was anti-conformation each other. It was then modified into eclipse conformation through 180^o rotation, to have the dihedral OH/OH, H/H corner turns from $180^o$to 0^o, and (iv) changing molecular rotation orientation which refer to Fischer projection. The correct answer is B, but what needs to be observed from the result of this study is that 80% students tended to select option D and E proportionally. What are dominant factors contributing into student's difficulty in interconverting dimensional structure to Fischer projection?

Following is an example of rationality for those selecting option D and E, in **Figure 6a** and **b.** Reasons described in **Figures 6a and b** show that both were initiated by proper ways of thinking; *i.e.* observing dimensional structure, finding main carbon framework, and numbering it. Afterward, however, there was some inaccuracy in transformation stages from dimensional structure to Fischer projection. In **Figure 6a**, the inaccuracy was on observer position. The written description tells that OH cluster in C number 2 is on the left and H is on the right of Fischer projection. It suggests that the observer considered that C number 1 was directed toward him. Such consideration is conflicting since it contravenes the rules. The observer should have set himself in such a way that C number 1 was directed backward or away from the observer. It all suggests the inaccuracy in interpreting the notation of full wedge and dash, the relation among them, and the implementation of rules to transform dimensional structure to Fischer projection. The rationality presented in **Figure 6b** indicates the accuracy of observer orientation, but insufficient attention or awareness to the rules of spatial arrangement or spatial orientation of clusters around chiral carbon atom in the Fischer projection. Both reasons exposed to seem to move all clusters on the left easily, located on the left of Fischer projection and *vice versa*.

The interpretation of vertical and horizontal lines in Fischer projection and its implication to the space was not considered properly. The result of the study shows that 80% students had such problems. These results support research by Olimpo[13], which reported that student in their study have difficulty in translating from Dash-Wedge to Fischer projection, since the students' lack of or incomplete understanding of the dynamic nature of molecules, as well as difficulty employing mental rotation techniques to translate between different representation of the Dash-Wedge and the Newman Projection. This account is in line with other researcher's ideas [7,8] that the use of 2D symbolic representation, such as Fischer projection, to visualize 3D representation and conversely is an intricate task and demands comprehensive skills to interpret it.

In this study, to supplement the data in addition to the test results, students were also given a questionnaire in order to reveal a learning process has been followed. Based on the results of the questionnaire, it was revealed that the implementation of the strategy in the lecture on the topic chirality which has lasted less involving students in constructing a concept, yet to optimize the use of a molecular model as media, both static and dynamic, as well as the lack of the task to interconversion between representations. This is believed to contribute to the comprehension ability of students in a 3D representation of the molecule and its interconversion on the topic chirality.

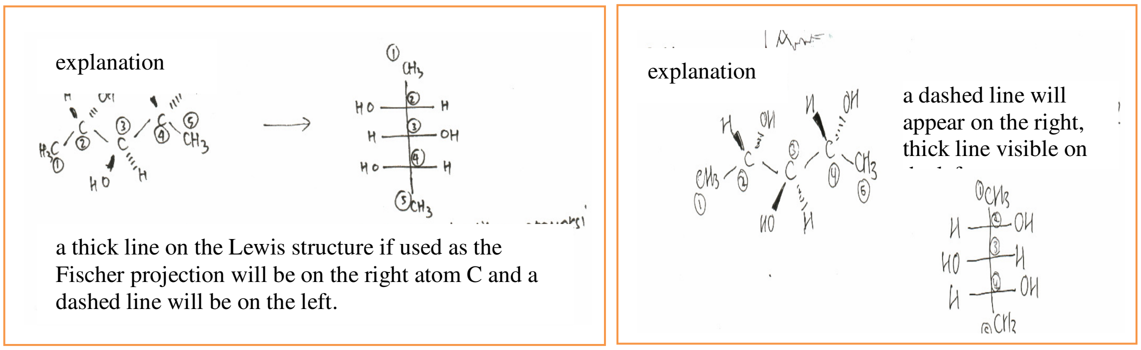

FIGURE 6 (a). An example of student's rationality for selecting option D; (b). An example of student's rationality for selecting option E, in test item number 5

CONCLUSIONS

This study reveals that in molecular chirality lesson, most teacher-candidate students were dealing with difficulties to comprehend 3D representation and its interconversion. The level of difficulty in comprehending inter-conversion among representations higher than 3D representation; multiplied complications. Dominant factors contributing to those difficulties were the inability to orient oneself as an observer, fragile operation of rotation, low spatial mindfulness, and improper consistency to implement symbols, rules, and relations among representation. This study recommends that learning shoud show more rigorous spatial awareness training tasks accompanied by the use of dynamic visualization media of molecules associated with the using of static molecular models to help students overcome the difficulties they encountered. [12] In addition, the result of this research is highly important taken into account that textbook and other forms of media in context of 3D molecule representation and its interconversion on chirality that frequently causes students' misconceptions reagrding diagrams, as they had been reported by Kumi.[14]

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