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In-House Training of 3D Molecular Modeling using Avogradro for High School Chemistry Teachers

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Abstract: The purpose of this activity is to improve the knowledge and skills of chemistry teachers in visualizing 3D molecules. This activity was attended by 20 high school chemistry teachers in Bandar Lampung. Methods in the activities include presentations, discussions, questions and answers and guided practice, and independent exercises. The results of the activity evaluation were revealed through questionnaire responses by the trainees as well as participant performance assessments which were revealed through the product of a 3D molecular structure visualized through the use of software. Avogadro. Based on the analysis of participants' responses, all participants agreed and strongly agreed that the Avogadro software opened an application that helped visualize 3D molecules; easy to operate; assist in teaching topics related to molecular shapes and carbon compounds, molecular properties with an attractive and dynamic appearance; provides a new experience that helps better understand the arrangement of atoms in 3D space. Based on a performance assessment in the form of a 3D molecular structure visualization product, all participants are skilled at visualizing a 3D molecular structure. Based on the results of the activity, it can be concluded that this activity can improve the knowledge and skills of high school chemistry teachers in Bandar Lampung in visualizing molecules in 3D with Avogadro software.

Keywords: molecular visualization, Avogadro, high school chemistry teacher.

▪ INTRODUCTION

Chemistry is a branch of science that studies the composition, structure, properties, changes in matter and the energy that accompanies these changes. To study the "structure" of matter, of course, cannot be separated from molecules. Molecules exist as three-dimensional structures and further “chemical behavior is determined by molecular structure” (Morrison & Boyd, 2002). On this basis, in learning chemistry from elementary to advanced levels, it is appropriate to explore the basic relationship between the three-dimensional structure of molecules and their properties (Hehre, Nelson, & Shusterman, 1998).

However, based on the results of preliminary studies through interviews with chemistry teachers at Bandar Lampung High School in learning chemistry for chemistry learning topics that require visualization of molecules such as particles of matter, chemical bonds, compound polarity, molecular shape, isomerism of carbon compounds to phenomena in microscopic level during chemical reactions, has not been able to accurately visualize the molecular structure. Teachers generally describe molecules in two dimensions. For students, learning how to interpret molecular structures visualized as simple line drawings is one of the biggest hurdles students face, and is one of the main reasons why many students find it difficult to study chemistry (Hehre, Nelson, & Shusterman, 1998).

For this reason, learning strategies related to 3D molecular visualization need to be optimized by utilizing relevant learning media. Some teachers have tried using the traditional ball and stick, or molymod, but this atomic model has many drawbacks including it takes a long time to assemble, and the comparison of atomic size visualization is not accurate. Unable to inform quantitative aspects such as bond length, bond angle. Plastic models in general do not help us identify the 'correct' molecular geometry (Hichliffe, 2003).

In addition to the molymod atomic model, computerized molecular visualization and modeling programs are currently available and can be accessed through open source internet sites. The advantages of using computer programs include showing accurate structures so that users can obtain information on atomic positions, atomic volumes, along with interesting features (Hahre, Nelson, & Shusterman, 1998; Pranowo, 2011). Thus, computers are more than just a simple structure display tool, but provides a means of visualizing, investigating, and studying various chemical phenomena. This advantage implies that the use of computer modeling is good for teaching the structure and properties of molecules.

Many research reports that describe the impact of learning using computer programs can help students (Tuvi-Arad & Gorsky, 2007, Abraham et al., 2010; Springer, 2014). Generally researchers report that a 3D drawing program helps students overcome difficulties in three-dimensional visualization, contributing to an in-depth understanding of the molecular structure and elements of complex molecular symmetry that are generally inaccessible from drawings. 2D, understand the concept g is abstract and at the microscopic level (Gilbert, 2005).

One of the software that is able to visualize 3D molecules accurately is the application of chemical structure drawing software such as Avogadro Software, which can bedownloaded via the internet site. http://avogadro.openmolecules.net . The reason for choosing software , apart from the availability of structure drawing facilities, software Avogadro Extension menu, which defines a plugin interface. Extensions properties dialogmolecule. Thus this software in addition to accurately visualizing 3D molecules,

but also provides facilities for a set of properties for the molecules that have been described.

Thus, to overcome the problem of the limitations of chemistry teachers in visualizing 3D molecules, a systematic guided training is needed which aims to introduce teachers to the Avogadro software application, so that they are skilled at operating and can use optimally as a medium for learning chemistry in high school. This training can be accommodated in a Community Service activity, it is hoped that through this training the insight and skills of the teachers will increase. This increase can be measured through the teacher's skills to visualize 3D molecules as well as get information on properties through the properties menu facilitated by Avogadro software. This activity aims to improve the skills of chemistry teachers in visualizing molecules in 3D.

▪ METHOD

The training activities were carried out for Chemistry teachers in Bandar Lampung. In this case there are as many as 20 participants involved. This small number of participants is because the implementing team expects the training to be effective and conducive. The method of activity is carried out through several steps, namely presentations and discussions by delivering material intro to computational chemistry which contains the basic concepts used in the Avogadro software. After that, it was continued with the practice of operating the Avogadro software, then exercises to give participants the opportunity to skillfully model the 3D molecular structure using the Avogadro software. Evaluation was carried out at the end of the activity to find out how the participants' understanding of the use of Avogadro software was increased to model 3D molecular structures. The evaluation instrument used was a response questionnaire to determine the participant's response to the insights and the importance of using Avogadro software as a tool capable of modeling 3D molecular structures. To measure participants' skills in describing 3D structures using Avogadro software, it was measured through the quality of the 3D structure images made by participants.

▪ RESULT AND DISCUSSION

Participants' responses to the 3D molecular modeling training using *software* Avogadro

At the end of the activity, the participants' responses to the 3D molecular modeling training using a questionnaire. Participants were asked to state their agreement (SS=strongly agree, S=agree, TS=disagree, and STS=strongly disagree) on each item of the questionnaire. The responses of the trainees are presented in Table 1.

Table 1. Responses of the trainees in 3D molecular modeling using Avogadro

No.	Statement	SS (%)	S (%)	TS (%)	STS (%)
1	Software “Avogadro” opens up insight into the existence of applications that really help visualize 3D molecules	90	10	0	0
2	Software “Avogadro” is quite easy to operate	75	25	0	0
3	Software “Avogadro” helps in teaching topics related to molecular shape and carbon compounds	40	60	0	0
4	software helps understand molecular properties in an attractive and dynamic way	80	20	0	0

5	Modeling with Software Avogadro atoms in 3D space.	30	70	0	0
6	I am enthusiastic about participating in this training because it helps me to easily draw 3D molecules.	80	20	0	0
7	I am interested in applying software in learning at school.	60	40	0	0
8	If this training is continued, I am interested in participating because it helps me improve IT literacy in learning.	75	25	0	0

Based on the information obtained from Table 1, it was revealed that 90% of participants stated Strongly Agree and 10% Agree, that the existence of the Avogadro software has opened participants' insight into applications that are very helpful in visualizing 3D molecules. This means that through this training, there has been a change in the teacher in the form of increasing insight between before training and after training. Before the training the participants did not have insight, but at the end of the training, the software really helps visualize the 3D structure of molecules. The teachers also strongly agree (75%) and agree (25%) that the software is quite easy to operate. This participant's response provided information that during the training process using the software, teachers can follow the steps in the training guide which contains the use of icons and menus available in the software to create 3D molecular images without any major difficulties. This condition is understandable, because during the training process, participants receive intensive guidance from the team, and if participants ask questions due to unclear stages or are hesitant when operating the software, the team immediately helps so that participants can immediately advance to the next stage of drawing.

Information on increasing teacher insight into the importance software can be used as a medium in teaching high school chemistry topics, obtained from the teacher's response to item 3. There are as many as 40% of teachers stating strongly agree, and 60% agree, that software helps in teaching topics -The topic of chemistry is related to the shape of molecules and carbon compounds. This data provides information that teachers feel confident about the relevance of the facilities available for drawing in the Avogadro software and the need for 3D structures that must be visualized when teachers teach topics related to molecular shapes and structures of carbon compounds. Participants' responses stating that they strongly agree (80%), and agree (20%), that the Avogadro software helps understand molecular properties, with an attractive and dynamic display providing information that trainees are skilled at operating menus and icons available to explore a set of properties. for the 3D molecule depicted. Through the “properties trainees can explore various physical properties of 3D structures, such as polarity and molecular energy. This information certainly cannot be obtained through molymod as a medium.

The responses of participants who stated strongly agree (30%), and agreed (70%), that Modeling with Software is a new experience that helps better understand the atomic order in 3D space, confirmed that the previous trainees were not familiar with the Software Avogadro. This means that there is a change in the form of increasing knowledge from not knowing. In addition, participants also stated that they strongly agreed (80%), and agreed (20%), that they were enthusiastic about participating in this training because the participants gained new experiences in the form of easy modeling of 3D molecular structures which were originally abstract and difficult to visualize.

The teachers also strongly agreed (60%) and agreed (40%) to apply software in learning in schools for topics relevant to the visualization of 3D structures. This is what the Team

hopes for in this training, so that the participating teachers can implement the results of the training, not only in training activities. The enthusiasm of participants to take part in the training at the next stage related to the use of Avogadro software for energy calculations and predicting molecular stability, was obtained from the responses of participants who stated strongly agree 75%, and agree 25%. This enthusiasm turned out to be related to the participants' belief in the needs of teachers in improving IT literacy. This statement provides an opportunity for the Team to continue similar training, introduce various other features of the software in addition to its ability to draw 3D structures and provide information on properties. However, the advantages of this software are also equipped links to quantum mechanics-based chemical computing software such as NWCHEM (Hanwell et al, 2012).

Product profile training Molecular 3D modeling using *software* Avogadro

The stages of preparation for the 3D drawing of molecules by the teacher, starting with downloading and then installing software open-source Avogadro. The icon is recommended to be stored on the desktop so that it is easy to find when it is used. Meanwhile, the display of the Avogadro software is presented in Figure 1, as follows:

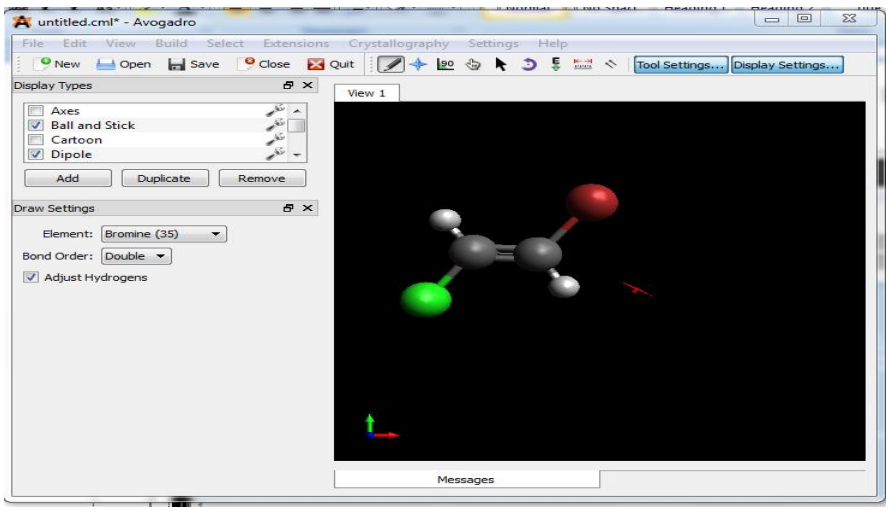
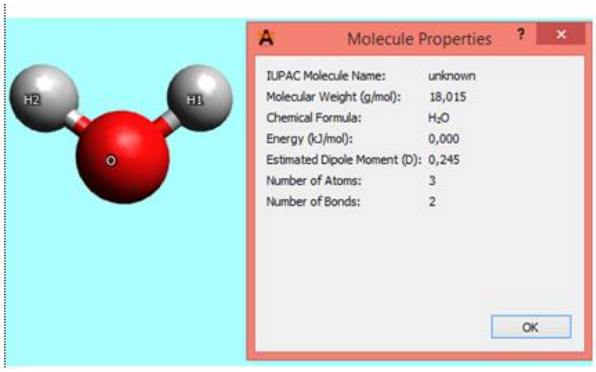


Figure 1. Display software Avogadro

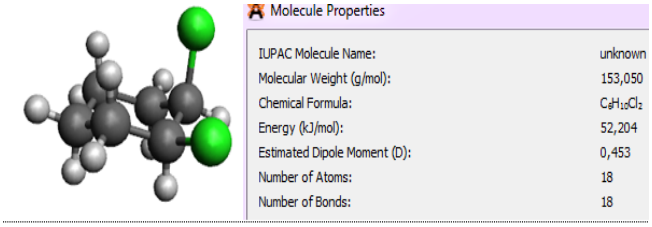
With this software, users can visualize 3D molecular images by clicking on the icon. At first, by clicking on this icon, the user will get an image of methane. For further drawing, the user can be creative according to the target molecule to be drawn.will appear the draw settings respectively which is useful for image settings, there is a menu for selecting the type of atom, selecting the type of bond, and adding atoms automatically. The 20 trainees, after being guided by the team to understand the guidelines for drawing molecular structures and their properties, were then assigned independently to practice drawing 3D structures and visualizing the resulting images.

In Figures 2(a),(b) and (c) the product of the trainees is presented in the form of visualization of the molecules assigned in this training. The molecular visualizations are designed in such a way as to be relevant to the teacher's needs in learning, namely 3D visualization (i) simple molecules that are very familiar to students such as H_2O, CO_2, NH_3, and methane molecules; (ii) visualization of molecules that contain double bonds and allow the emergence of geometric isomeric phenomena, and (iii) cyclic molecules,

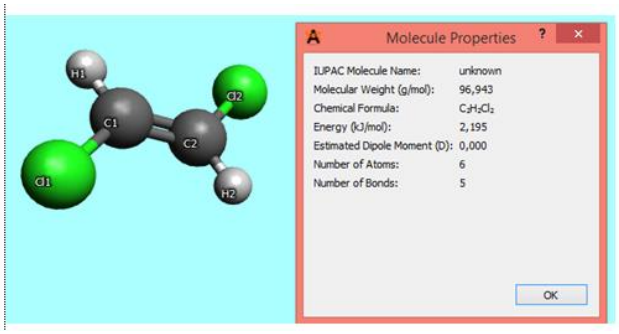
which are generally presented in textbooks as two-dimensional images which often lead to misconceptions, that cyclic molecules are flat molecules. (Abraham et al., 2010).



(a)



(b)



(c)

Figure 2. (a) An example of modeling a simple molecule (H_2O), (b) an example of modeling a substituted cyclohexane molecule, (c) example of modeling a molecule containing a double bond

The visualization shown above is done by copying the image on the Avogadro software display page, then saving it in doc format. The assessment by the team is based on the file sent to the team leader's email address. The assessment of the 3D structure product that has been drawn by each participant is based on a rubric. The rubric components include (i) the suitability of the visualization with the name, (ii) the image is the result of geometric optimization, (iii) the clarity of the arrangement of atoms in space, (iii) the clarity of the differences between conformers/isomers, and (v) the proportion of image sizes. The results of the product assessment visualized by the 20 trainees are presented in Figure 3.

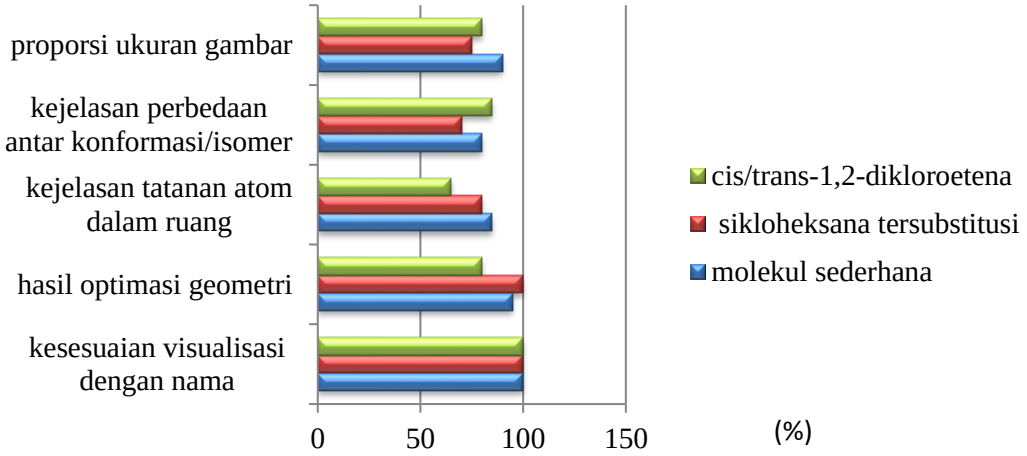


Figure 3. Product quality profile of visualization of the 3D molecular structure by the trainees

In Figure 3 above shows that the trainees have been skilled at drawing 3D molecular structures through Avogadro software. there are 5 criteria for assessing the visualization of 3D structures using Avogadro, namely (1) the suitability of the visualization with the name of the structure being studied; (2) the visualized molecular structure has gone through the geometry visualization stage; (3) clarity of the shape of the atomic arrangement in space, (4) clarity in the different types of conformation/isomerism; and (5) the proportion of image size to screen size. The results show that in the assessment criteria (1), all trainees successfully and skillfully use the menus in the *software* in terms of atom selection, bond order, making cyclic structures, and adding hydrogen atoms. On the assessment criteria (2); intended to check that the created image has gone through geometry optimization or not. Through the *optimize geometry menu*, the initial image created will then be optimized in terms of angle size parameters, bond lengths, and atomic arrangement in space that is close to the real structure.

▪ CONCLUSION

Based on the description of the evaluation results of service activities, it can be concluded that there is an increase in the knowledge and skills of chemistry teachers at SMA Bandar Lampung in visualizing molecules in 3D with Avogadro software.

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