USE OF A MOLECULAR VISUALIZATION FREE SOFTWARE IN A CHEMISTRY MODULE

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Abstract

There seems to be a widespread perception amongst researchers and teachers that many students find chemistry difficult [1]. Having a good knowledge of molecular structure is crucial to work out polarity of compounds, intermolecular forces and their relationship with properties. In addition, it is very important to understand the inorganic systems that explain the behaviour of atoms, ions and molecules in understanding the phenomena of organic chemistry [2]. Therefore, the understanding of spatial structures is central to the discipline of chemistry. However, in textbooks molecular structures are represented as two-dimensional objects and as result, students might find difficult to switch from 2D to 3D structures or images. Using 3 dimensional models help students acquire a better understanding of molecular geometry and encourage active learning. Computer visualizations now offer an interesting possible alternative to concrete or physical models [3]. Jmol is one of the most prevalent molecular visualization tools in STEM education. It is a free open source software for interactive molecular visualization. This work describes the implementation of the Jmol visualization tool in a module on General Chemistry for Engineers during the academic year 2016-2017. The goals were three-fold. Firstly, to use the Jmol visualization application as a teaching tool for classroom demonstration. Then, to provide students with the skills to use the molecular visualization tool for their own learning process. Finally, to actively engage students with generation and manipulation of molecular models. Jmol application was used during Lectures to teach about molecular structure. Students then had to download and use the application on their own to complete several worksheets. Later on, Jmol molecular models were also used to aid student understanding of organic chemistry, including isomerism. Additional worksheets and assignments involved the use of Jmol visualization tool. The evaluation of the software implementation on the module was carried out by marking the worksheets and by a survey that was conducted among the students.

Keywords: 3D molecular models, Jmol software, organic chemistry.

1 INTRODUCTION

There seems to be a widespread perception amongst researchers and teachers that many students find chemistry difficult [1]. One of the major reasons is that chemistry topics are very abstract. Chemical bonding and molecular structure are some of the key concept areas in this subject, and are also areas where learners are known to commonly acquire alternative conceptions or misconceptions. These misconceptions have been researched under the categories of bond polarity, molecular shape, polarity of molecules, intermolecular forces, etc. [2]. Having a good knowledge of molecular structure is crucial to working out polarity of compounds, intermolecular forces and their relationship with properties. In addition, it is very important to understand the inorganic systems that explain the behaviour of atoms, ions and molecules in understanding the phenomena of organic chemistry [3]. That is, to gain knowledge about organic chemistry, students need to have developed an ability to visualize molecules in three dimensions [4]. Therefore, the understanding of spatial structures is central to the discipline of chemistry. However, in textbooks molecular structures are represented as two-dimensional objects and as result, students might find difficult to switch from 2D to 3D structures or images. Using 3 dimensional models help students acquire a better understanding of molecular geometry and encourage active learning. Computer visualizations now offer an interesting possible alternative to concrete or physical models [5]. Students tend to look upon the concrete models as a reproduction of reality and not as constructed images. Computer visualizations, on the other hand, can be handled like real models without being or ever seeming real [6]. They offer additional advantages: they allow molecular models to be displayed in front of a wide audience and the use of diverse representations of a molecule: wireframe, ball and stick, space-filling, sticks. The models are
interactive, in the sense that the user can choose all sorts of actions to be performed on the model [7]. Animation can add considerable learning potential to computer-generated visualization. For example, by rotating a molecular model, one can get a better appreciation of its 3D structure. This software interactivity can increase active students’ involvement; we are allowing them to discover certain aspects of chemistry on their own. Jmol is one of the most prevalent molecular visualization tools in STEM education. It is a free open source software for interactive molecular visualization. Since Jmol is written in Java programming language, it is compatible with all major operating systems.

2  OBJECTIVES

This work describes the implementation of the Jmol visualization tool in a module on General Chemistry for Engineers during the academic year 2016-2017. This module belongs to the Bachelor of Science in Industrial Engineering offered in the Engineering School of Bilbao (University of the Basque Country, UPV-EHU). The goals were the following:

- To use the Jmol visualization application as a teaching tool for classroom demonstration.
- To provide students with the skills to use the molecular visualization tool for their own learning process.
- To actively engage students with generation and manipulation of molecular models.

3  METHODOLOGY

"General Chemistry for Engineers" (GCE) is an undergraduate core module for 1st year of Bachelor of Science in Industrial Engineering for different engineering branches: Electrical, Mechanical, Electronics. It is a 9-ECTS module and it is a full year module. It is offered in Spanish, Basque and English. This is a core module that aims to provide students with knowledge of basic chemical principles and theories about properties and performance of matter. The teaching methods are lectures (2h/week) during the first term and in the second term in addition to the lectures, there are seminars and laboratory sessions. Topics covered by the syllabus include atomic structure, chemical bonding, intermolecular forces and organic chemistry. The three main types of chemical bonding are studied (ionic, covalent and metallic) and their properties are discussed. Intermolecular forces between molecules and the resulting properties are described. The goal of the unit on Organic Chemistry is to provide students with foundational concepts. It introduces naming conventions, main functional groups, isomerism and organic reaction terminology. Isomerism is the phenomenon whereby certain compounds, with the same molecular formula, exist in different forms owing to their different organizations of atoms. The concept of isomerism illustrates the fundamental importance of molecular structure and shape in organic chemistry. Participants in this study were students enrolled on the “General Chemistry for Engineers” module.

4  PROCEDURE

4.1  Design and implementation of the Jmol visualization tool

The implementation took place in several steps. Firstly, during the Lectures on the topic of molecular structure Jmol was introduced to show students the different types of simple molecular geometry. The notes available for students included images of molecular structures from Jmol. Part of a lecture was used to show them how to start using the application and become familiar with it. They were introduced to working with the model kit option to build molecules, learnt how to perform simple measurements such as bond lengths and bond angles, rotating molecules, changing the style, etc. Then, students were given instructions to download and start using Jmol software on their own laptops. In order to promote the use of this visualization software, they were given worksheets that required the use of Jmol. Students were asked to draw the Lewis dot diagrams of different molecules and apply the VSEPR model to predict the more stable geometries or shapes. Then, they were asked to build those same molecules on the Jmol application to check their predictions and to measure the bond angles and lengths. Fig. 1 displays a snapshot of a Jmol session.
They also had to deduce both the bond polarity and molecular polarity, identify the intermolecular forces and rank properties such as melting and boiling points for related compounds on the basis of these forces. By introducing the Jmol software early in the course, the students had become familiar and used to working with the visualization tool by the time the topic of organic chemistry was introduced. Jmol visualization tool was applied to illustrate the different types of hydrocarbons: alkanes, alkenes and alkynes, cycloalkanes and aromatic compounds. The concept of isomerism was also illustrated with the help of Jmol models, different compounds having the same molecular formula were discussed in the classroom. Then, students were given home assignments where they had to use Jmol to perform tasks of increasing levels of difficulty. The first ones demanded to build organic molecules of aliphatic and aromatic hydrocarbons. Later on, students had to think about and work out the isomers for a given molecular formula and show them in Jmol.

4.2 Evaluation

Students were introduced to Jmol software during one lecture. After teaching them the basic steps to build molecular models and to manipulate them, they were asked to download the free software and start using it. Then, they had to submit several assignments that consisted of worksheets. These worksheets activities were marked and students were provided with feedback. Additionally, after the implementation of the visualization software, students were asked to fill in a final survey. It was meant to check whether students had found the use of this software tool useful.

Table 1. Organic Chemistry worksheet example

1. Make the models of methane (CH₄), ethane (C₂H₆), propane (C₃H₈) and n-butane (C₄H₁₀). Observe that all of the bond angles are equivalent (measure the bond angles). Measure the bond length.
2. Make the models of cyclopropane (C₃H₆), cyclobutane and cyclopentane. Do you think these are highly stable molecules?
3. Make cyclohexane (C₆H₁₂). Note the conformation.
4. Add 3 double bonds to make the model for benzene (C₆H₆). What is the conformation for benzene?
5. Make the models of CH₂CH₂ and CHCH. Measure their bond lengths. What is the shape of each molecule?
6. Make a model of n-butane (C₄H₁₀) and isobutane (C₄H₁₀) or 2-methylpropane. Note that they are structural isomers and chain isomers since they differ in the position of the C atoms. Both models display different molecules with different properties. Look up the density, boiling point and melting point for n-butane and isobutane.
7. Make the model for pentane C₅H₁₂. There are three structural isomers for C₅H₁₂. Make a model for each one.
8. Make a model of propane and replace one hydrogen atom by a chlorine atom: \( \text{C}_3\text{H}_7\text{Cl} \). There are two molecules with that same formula. Make both models.

9. Make the model for butane and then work out and make the models for the isomers with the formula \( \text{C}_4\text{H}_9\text{Cl} \).

10. Consider the molecular formula \( \text{C}_2\text{H}_6\text{O} \). There are two compounds that correspond to this formula: ethyl alcohol and dimethyl ether. Make their models. These are structural isomers, they display the same molecular formula and in this case different functional group.

Table 2. Final survey

Q1. Have you taken any Chemistry modules before?
If you have: Q2. During how many years? And what grades?
Q3. Did you learn about Organic Chemistry? And isomerism?
Q4. Have you used any visualization software tools before?
Q5. Please rate the following sentences on a scale of 1-5:
   1. Installing Jmol application was easy
   2. The instructions for using Jmol software application were clear and understandable
   3. The use of the Jmol application was useful to understand molecular visualization
   4. I have become familiar with using software tools to create visual representations of molecules.
   5. The assignments and worksheets were helpful to visualize molecules in 3 dimensions

5 RESULTS AND DISCUSSION

Students showed interest when they were introduced to the software application and they expressed willingness to start using Jmol. The marking of the assignments showed that most students worked very well and used the Jmol accordingly. The difficulty level of the assignments was increased gradually. At the end a survey was conducted (table 2). According to their answers to Questions 1 and 2, all students had enrolled for Chemistry modules before; most of them had studied Chemistry for two years during Baccalaureate. However, not all of them had studied Organic Chemistry. Answers to Question 4 showed that no student had used any visualization tools before. The ratings to Question 5 are displayed in Fig. 2.

**Figure 2. Results from the students’ answers to Question 5**
This question included five categories or statements. The answers were given in a 5 point scale (1- strongly disagree to 5-totally agree). The average responses to these categories were the following ones: 4.3; 4.7, 4.7, 4.7, and 4.3. According to answers to categories 1-2, students found that installing Jmol free software was easy and agreed that the instructions provided were clear and understandable. This is a positive result in the sense that the installation and the instructions posed no special problems at the beginning of the implementation process. Results to category 3 clearly stated that Jmol was useful to understand molecular visualization. Similarly, the ratings to category 4 showed that students considered that they had become familiar with using visualization tools. In a slightly lower rating, they also agreed with category 5 statement, about the usefulness of the assignments.

6 CONCLUSIONS

The Jmol virtual learning environment was applied during a foundation chemistry module. It was used as a teaching tool for classroom demonstration both for learning about covalent bonding of inorganic molecules at the beginning of the module and about organic chemistry later on. This software was also intended to provide students with the skills to use it for their own learning process and the results obtained assessing the assignments showed this to be the case. Besides, students displayed a very positive attitude towards the visualization tool. Similarly, this experience was meant to engage them with the generation and manipulation of molecular models. Through both the assignments and their answers to the survey questions it could be said that this goal was also achieved. The results reported show that Jmol free software has been a useful tool.

REFERENCES


