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How Chemicals' Drawing and Modeling Improve Chemistry Teaching in Colleges of Education

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Abstract Our assumption states that integrating chemical drawing and modeling tools in teaching could promote chemistry teaching at the college level, and therefore improve the ability of students in colleges of education to understand better chemistry. During the last academic year, we incorporated CHEMDRAW software and tested how it affects students' performance in the exams. The improvement in the averaged score from 5.7 (prior CHEMDRAW incorporation) to 7.73 (post CHEMDRAW incorporation) clearly reveals that integrating modeling tools in chemistry education is helpful. The students' feedback following the initiative was positive and very supportive. Most students stated that with CHEMDRAW, they experienced a challenging learning environment engaged with dynamic illustration & interactive visual and would like to see such software integrated in their chemistry studies from day one. In the future we aim to test other parameters, e.g. Students' attitude toward learning chemistry as well as in more depth students' conceptual understanding in chemistry.

Keywords: *chemical education, computer-based learning, chemical drawing, CHEMDRAW, molecular properties, molecular structure*

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1. Introduction

Chemistry can be described at three distinct levels; namely, a) the macroscopic level (visible/touchable phenomena), b) the microscopic level (atomic/molecular), and c) the symbolic level (representing matter in terms of formulae and equations) [1]. Students who are studying chemistry are supposed to think at the microscopic levels and explain changes at the macroscopic levels [2]. Students are supposed to link 2D and 3D structures of chemicals to their physical properties [such as the physical state (gas, liquid, or solid), the appearance of the chemical, boiling & melting points, density, state at room temperature, and color] and chemical properties (Enthalpy of formation, Flammability, Preferred oxidation state, Coordination number, etc.). All of these think should be "cooked" in mind.

Lecturers in most colleges of education still use textbooks and 2D pictures to illustrate molecules. Many researchers claim that the use of still pictures enables building of a mental model of new concepts and phenomena, while others claim that still pictures are not adequate and utilizing animated pictures is MUST for promoting conceptual understanding [3]. Chandrasegaran and his colleagues [2] claim that students' ability to use macroscopic, microscopic, and symbolic representations is necessary for understanding chemistry concepts and phenomena. Students who are studying chemistry are requested to think at the microscopic level (in terms of interactions between individual atoms and molecules) and explain phenomena at the macroscopic level [4]. According to Chandrasegaran [2], students find it difficult to properly connect between the different levels of understanding. It seems that students don't have adequate understanding of the macroscopic/microscopic representations of molecules and the meaning of the symbols and formulas in chemical equations. These difficulties, along with the difficulties in understanding the 3D structures of molecules, hinder students' ability to solve problems in chemistry. Science educators proposed several solutions to overcome these difficulties, such as: integrating three dimensional visualization tools, and promoting the switch between different chemical representations [5].

Researchers have found that integrating visual representations such as computerized molecular models, simulations, and animations in teaching may promote students' understanding of unobservable phenomena in science [6], and afford them with the opportunities to make abstract concepts visible. Manipulating chemical structures in 2D/3D representations help students relate the macroscopic, microscopic, and symbolic representation levels of chemicals to each other [6] and enhance students' conceptual understanding and spatial ability [7].

There are many tools that enable students to manipulate chemical structure in either 2D or 3D representations, and build molecular models, Table 1 summarize some of such well-known computerized tools.

ChemDraw software is the drawing tool of choice for researchers to draw chemicals for publications/ presentations and for querying chemical databases. In most academic institutions, the program is used for drawing chemicals but not as a teaching tool. A version of the software for iPad was developed recently and Michael Lewis from Saint Louis University reported in EmergingEdTech [8] that they use it in classroom aiming to engage all students and give them an incentive to participate. The utilized feature of the software is the chemicals drawing feature. However, ChemDraw has a powerful set of tools that could be utilized in teaching, taking advantage of the set of tools to calculate/ predict chemical/ physical properties, generate spectra, construct correct IUPAC names, and calculate reaction stoichiometry.

Table 1. List of chemical drawing and modeling tools running on Microsoft Windows platform.

Software	Developer	Information
ChemDraw	Cambridge Soft	
Avogadro	Avogadro project team	3D molecule editor and visualize
Chem Window	Bio-Rad	Freeware for academic research and teaching
KnowItAll	Bio-Rad	Freeware for academic research and teaching
Accelrys Draw	Accelrys	freeware version available; includes name 2 structure and structure 2 name
ACD/ChemSketch	ACD/Labs	freeware version available
BALLView	BALL project team	viewer, editor and simulation tool
MedChem Designer	Simulations Plus	freeware - includes calculation of logP, logD (7.4), sigma charges, Hydrogen Bond Donors, Hydrogen Bond Acceptor
ICM-Chemist	MolSoft	Easy to use graphical user interface desktop chemistry editor
ChemDoodle	iChemLabs	
ArgusLab		Freeware
Ascalaph	Agile Molecule	Freeware
Amira	Visage Imaging Zuse Institute Berlin	14 day trial version available

2. Methods

Incorporation of ChemDraw in teaching

Nomenclature and molecular structure are most frequently the first topics students come across in organic chemistry. Students encounter problems in learning nomenclature from the chemistry textbooks and from the teachers [9]. ChemDraw software offers several features that allow students to efficiently learn such topics. By ChemDraw we convert chemical formulas and chemical names to skeletal structures and vice versa as well as skeletal/condensed structures to their corresponding IUPAC names [10]. Herein we give few practical examples:

We draw the following chemical

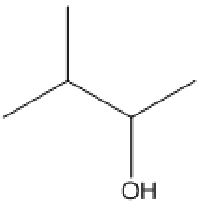

Figure 1.

And later clicking on the icon "convert structure to name". It gives:

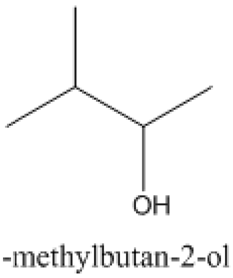

Figure 2.

As well we can convert names to structures. When we click on the icon to convert name to structure and wrote "2 methyl 2 propanol" it gives:

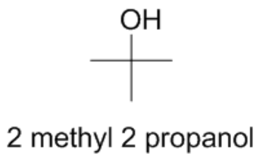

Figure 3.

With ChemDraw software, we can draw easily chemicals and predict their physical and chemical properties (Figure 4). This could enable students to well understand and interpret relationship between chemical structure and physical/chemical properties such as polarity, boiling point/ melting point and heat of formation. Herein we give a practical example revealing the relationship between boiling points of the alkanes/ lipophilicity and molecular size (or number of carbon atoms):

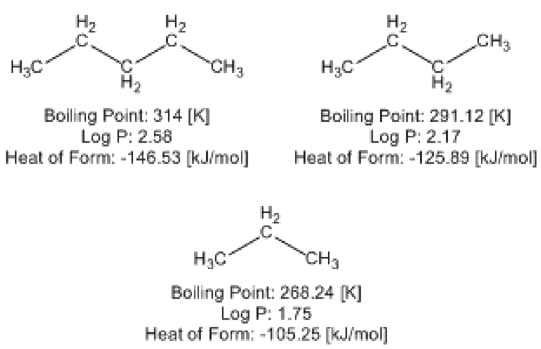

Figure 4. Drawing 2D structures of Propane, Butane, Pentane and predict their properties (such as Boiling Point, Log P, Heat of Formation). Log P is an index of lipophilicity showing the ratio of concentrations of a compound in a mixture of water and octanol. Low LogP means highly soluble in water. Lower Heat of Formation predicts more stable chemical. The student can figure out that there is a correlation between number of carbon atoms in alkanes and boiling point

As well as relationship between branching degree in alkanes and boiling point:

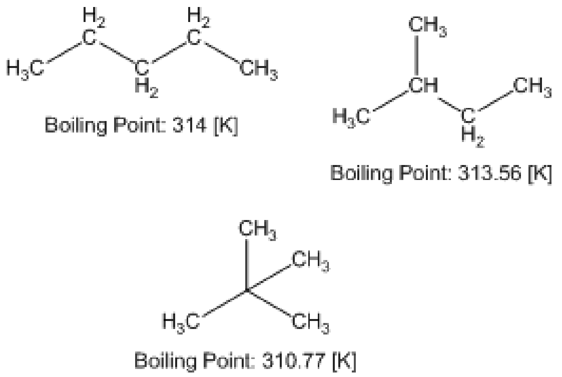

Figure 5. Drawing 2D structures of different isomers of alkane with molecular formula C_5H_{12} and predict their Boiling Point. The student can figure out that branching decreases boiling point. It is worth to assign that the stated boiling points are predicted ones and not the exact experimental boiling points

The students could internalize more properly some concepts such as “a molecule is in continuous motion” by practicing chemicals drawing & 3D modeling. As well they will be able to correlate between conformation and energy/stability and understand more better terms like van-der-waals and hydrogen bonding. Herein we give a practical example, demonstrating by converting two-dimensional structure to three-dimensional structure molecule in motion (different conformers having different types of interactions, leading to different energies and stabilities):

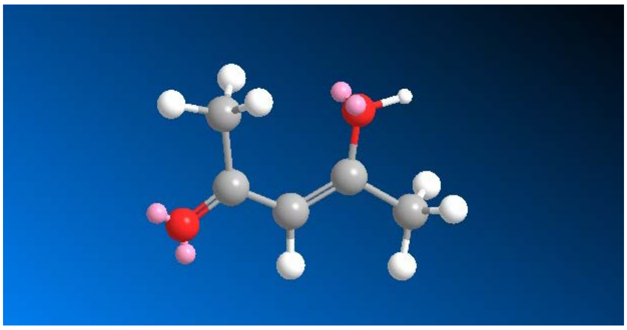

Figure 6. minimized conformer no. 1

Total energy is equal 3.7 kcal/mole. Intra-molecular hydrogen bonding is not exist. The proton donor is far away from proton acceptor. It is worth to assign that one of the crucial conditions to make hydrogen bonding interaction available is that the distance between proton donor and proton acceptor should be less than 3.5 Å.

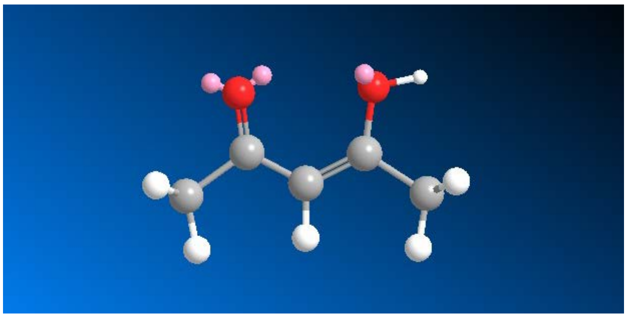

Figure 7. minimized conformer no. 2

Total energy equal 6.2 kcal/mole. The intra-molecular hydrogen bonding is not exist in this conformer as the hydrogen atom is pointing toward the opposite direction of the carbonyl oxygen atom and there is a repulsive interaction between both oxygen atoms due to electron lone pairs proximity. This repulsive interaction contributes too much to total energy increase.

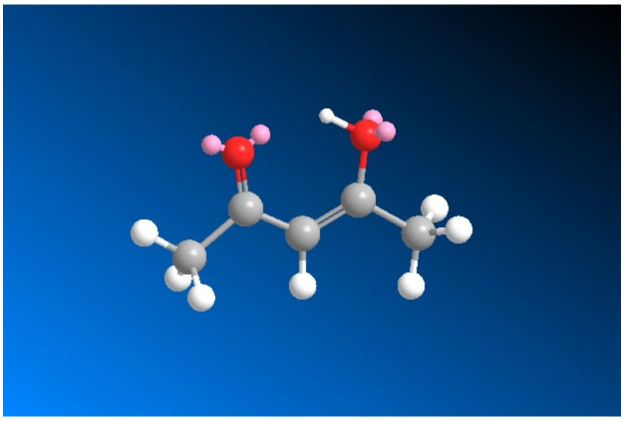

Figure 8. minimized conformer no. 3

Total energy equal -1.96 kcal/mole. The intra-molecular hydrogen bonding exists in this conformer and there is an attractive interaction between the carbonyl oxygen atom and the hydroxyl. This attractive interaction contributes too much to total energy decrease and stability of the conformer. There is a resonance and the proton could be shared between both oxygen atoms.

Our research population included students from Al-Qasemi academic college who are learning science courses (we have twenty eight students in total, first-year college students in science education department. Out of them, only 24 students took part in this research). Students were asked to consent to take part in the project in advance.

The dependent variable that was studied in this research is students’ performance in the exams. While, the independent variable was the teaching method (strategy) of chemistry in the college (i.e. teaching chemistry to college students with integrating CHEMDRAW as modeling tool, and teaching chemistry to college students without integrating any modeling tool).

3. Results and Discussion

Our main purpose is improving the quality of teaching chemistry in Al-Qasemi Academic College of education and making the learning experience more interesting and challenging by combining computerized modeling approaches & techniques with current teaching paradigm, providing new tools for active learning, interactive study environment and expanding sources of knowledge. We believe that incorporating in silico techniques may allow meaningful learning and give students a sense of security and capability of self-learning. Many studies indicate that traditional frontal learning is providing a mean for acquiring knowledge but it is kept only for a short time. However, the knowledge acquired under conditions of interactive study environment combined with senses of sight and sensing, may last for a longer times. In this way, the instructor main role is not only knowledge transfer for his students but sharing them active process of knowledge creation and acquisition.

Evaluation metrics are based on the results, which reflected in depth understanding of the concepts and implementation of studied material. These topics were tested with two exams accessed by students which included questions like:

- Three dimensional structures of chemicals & chemicals polarity.
- Relationships between melting/ boiling points and isomers' types.
- Converting names to two dimensional chemical structures.
- Converting two dimensional chemical structures to names.

Here are a summary of the initiative activities run during the 2nd semester of 2014 academic year:

- Prior workshop exam.
- Workshop: introduction for usage of CHEMDRAW software.
- Students' own practice (due to time limitation of this initiative, it was available only for few days).
- Post workshop exam.
- Results analysis.

Table 2, summarize the outcome, revealing that incorporating CHEMDRAW software in teaching chemistry aided in understanding some of the studied concepts, e.g. three-dimensional structure and polarity, boiling point and isomers structures, and implementation of AUPAC rules in converting chemical names to structures, and vise versa.

Table 2. How does incorporating CHEMDRAW software in teaching chemistry affect students' outcome in exams

Question Type	Average I (STDEV)*	Average II (STDEV)**	Improvement (STDEV)
Chemical name to structure	5.83 (2.22)	7.08 (2.39)	1.25 (1.98)
Chemical structure to name	5.33 (1.93)	7.96 (2.40)	2.62 (1.61)
3D structure & polarity	5.94 (2.21)	8.15 (1.94)	2.21 (1.89)
Total average	5.70	7.73	2.03

* Prior workshop exam ** Post workshop exam

Students' feedback

Upon completion of the initiative, students were asked for their opinion regarding the initiative and its contribution to their performance in the exam. The students said that with CHEMDRAW they experienced a challenging learning environment engaged with dynamic illustration & interactive visual and would like to see such software integrated in their chemistry studies from day one.

4. Conclusions

We came to the conclusion that integrating modeling tools such as CHEMDRAW software in chemistry education is helpful. The improvement in the averaged score from 5.7 (prior CHEMDRAW incorporation) to 7.3 (post CHEMDRAW incorporation) is very impressive. The students' feedback following the initiative was positive and very supportive. Most students stated that with CHEMDRAW they experienced a challenging learning environment engaged with dynamic illustration & interactive visual and would like to see such software integrated in their chemistry studies from day one. Other parameters could be tested in the future, e.g. Students' attitude toward learning chemistry as well as in more depth students' conceptual understanding of chemicals.

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