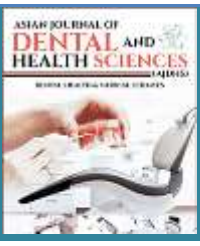

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Review on Molecular Modelling in Chemistry Education

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Abstract

Molecular models derived from results of quantum-chemical calculations present an important category of didactic instruments in chemistry education. These models can be used especially as tools for supporting the students' understanding by visual learning, which can adequately address complexity of many chemical topics, incorporate appropriate didactic principles, as well as utilize the benefits brought up by the actual information technology. The proposed molecular models are non-trivial examples of didactic application of computational chemistry techniques in illustration of electron interactions in amidic group, namely the interaction of the free electron pair on the nitrogen atom with the carbonyl group and also the interaction of atoms in the amide group with other surrounding atoms in the molecule. By these molecular models it is possible to explain acid-base properties of amides applying knowledge of electron density distribution in the molecules and the resulting electrostatic potential. Presentation of the structure and properties of the amides within education is important also for the reason that amidic functions are involved in many important natural substances (e.g. proteins, peptides, nucleic acids or alkaloids), synthetic macromolecular substances (e.g. Silon) or pharmaceutical preparations (e.g. paracetamol). This paper investigated the effect of using different types of models while teaching organic chemistry on student understanding of new concepts and the spatial structure of new molecules, as well as preference of a particular model type and illustrates the possibilities of computer-assisted molecular modelling in supporting chemistry teaching and learning.

Keywords: Molecular models, Acidity, Amides, Basicity, Electrostatic potential

Introduction

Chemical concepts are abstract by nature and therefore challenging to illustrate in an understandable way. The triple mode of representation brings more challenge to chemistry learning on the macro level, the submicroscopic level and the symbolic level[1]. At the macro level one can see and observe chemical phenomena. The submicroscopic level justifies and illustrates the visible properties of a substance with atoms, molecules and ions (for example with molecular modelling). The symbolic level shows the macro level and micro level phenomena using chemical symbols, formulas and equations. It is important that teachers understand the threefold relationship so that it can be conveyed to their students[2]. While a teacher moves smoothly from one level to another, a student might be confused and get a fragmented vision of chemistry. According to Gabel (1999), the primary barrier in understanding chemistry is that chemistry instruction occurs predominantly on the most abstract level, the symbolic level. The unobservable submicroscopic level, in which phenomena and concepts are difficult to be combined with the students' perceptions and the living environment, produces also problems for students [3]. Therefore students need to use different models, analogies or computer graphics to make invisible into visible[4]. Since models and modelling are essential in chemical thinking and in the development of scientific knowledge they should also be included in chemical education. Students should: learn about the nature of models and their usage as thinking tools; learn about the scope and the limitations of specific chemical models; be encouraged to use multiple models for a given phenomenon[5]. Visualizations help students to build mental models when learning about difficult concepts and submicroscopic level phenomena. That is why the students' visualisation skills, spatial ability particularly, should be developed. Computer-based molecular modelling has helped a variety of learners to improve their visualisation skills and helped them to understand the concept of the model, three-dimensional molecular structure and chemical bonds[6]. Molecular modelling software and computer-assisted learning materials enable new learning environments where chemistry concepts and phenomena can be viewed and perceived in a new manner. At the same time computer-assisted methods create new approaches enabling challenging chemistry topics to be clarified and simplified. Virtual models and visualisations can be modified according to the needs of teaching and learning[7]. Computer-based molecular modelling provides a tool for teaching and learning in order to support the visualisation of chemical phenomena and the development of chemistry teaching[8-11]. The computer enables to perceive things through visual experience which helps memorise things and improves learning outcomes[9]. According to the experiences of Finnish school teachers, computer-based molecular modelling helps teachers to illustrate and students to learn difficult concepts in chemistry in a new way, it develops students' visualisation skills and makes students interested in chemistry[12]. Finnish school teachers have used molecular modelling to illustrate the spatial structure of molecules, isomerism, atomic and molecular orbitals, chemical bonds, electron density, IR-spectroscopy, energy and its changes in chemical processes and chemical reactions. Molecular modelling can also be applied to biochemistry, biology and biotechnology education. According to Pernaa, Aksela and Lundell (2009) [10], high school teachers experienced that molecular modelling supports the drawing of conclusions and the understanding of three-dimensional structures and it provides added value for teaching of orbitals, chemical bonds and biomolecules. Teachers and students generally have positive attitudes towards molecular modelling[8, 12]. The teacher has an important role in the success and effectiveness of teaching chemistry through computer-based molecular modelling, because the use of modelling programs should not remain merely as a funny trick, instead working with a computer should be tied into teaching. The instructions and questions direct the learner's interest and activities in order to support learning tasks as well as it is possible and to train higher-order thinking skills[13]. The current learning theories highlight learning as a socially interactive process based on the students' experiences. By using computer-based molecular modelling it is possible to support the understanding of scientific concepts, practice different learning skills and to motivate students to investigate in an authentic research environment[9]. There are commercial molecular modelling programs e.g. Spartan (www.wavefun.com) and HyperChem (www.hyper.com), and free programs e.g. ChemSketch (www.acdlabs.com), ArgusLab (www.arguslab.com), Symyx Draw (www.symyx-draw.en.softonic.com), Avogadro (www.avogadro.en.softonic.com) and MarvinSketch (www.chemaxon.com). Edumol (www.edumol.fi) is an open, web-based environment for molecular modelling and visualisation. Findings indicate that molecular modelling has helped students to understand concepts in molecular geometry and bonding[8] as well as in model concept, isomerism and functional groups[14]. In the ongoing doctoral study, the meaningful teaching model for covalent bonds (as opposed to rote learning) is being developed.

Brief history of the development of molecular models

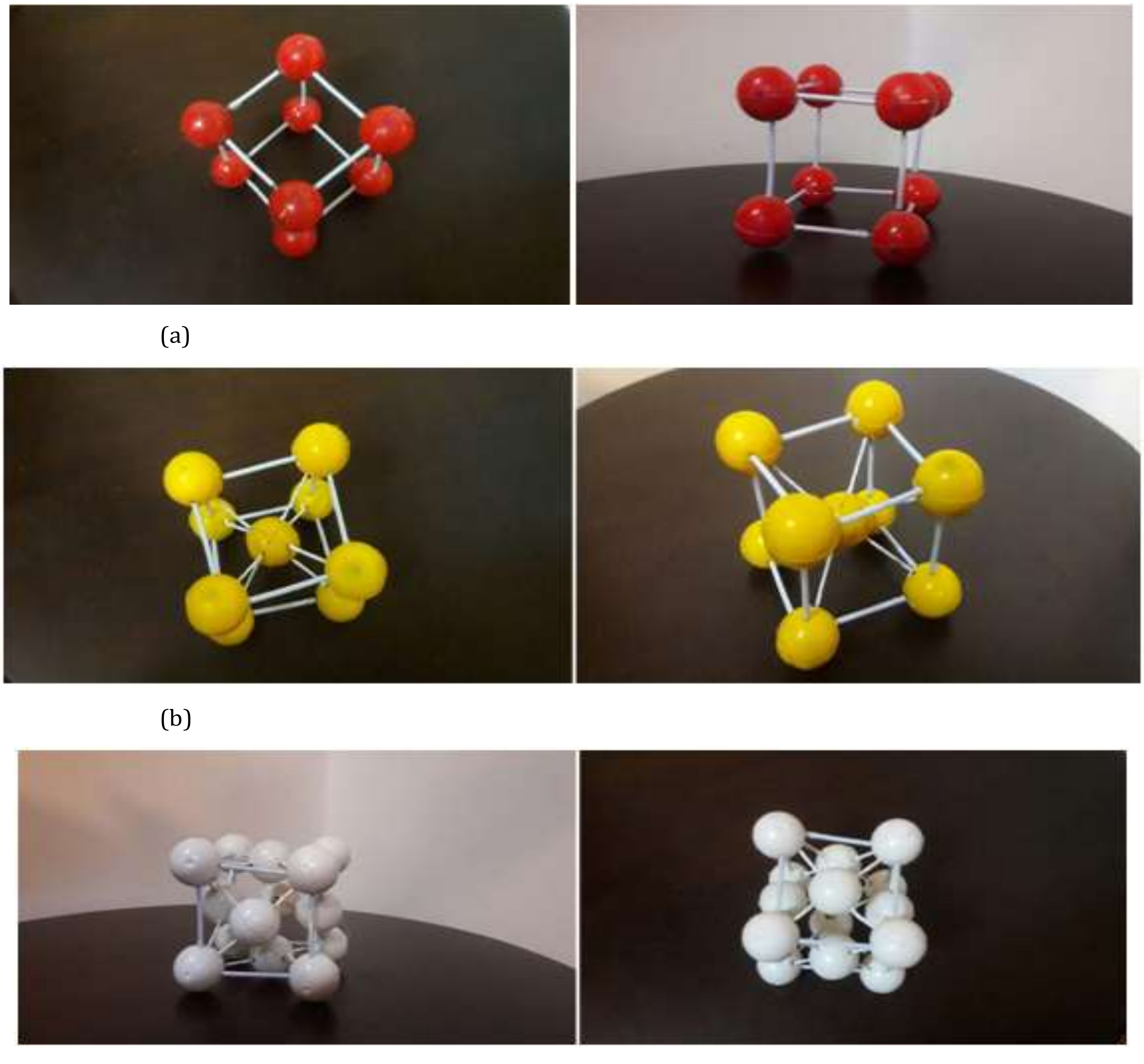
The history of models[15-18] can be traced back to Plato (482-347 BC), who conceived of the four elements- soil, water, air and fire. Nothing much happened in terms of model development until in 1808 Dalton published the *New System of Chemical Philosophy*- the first substantial discourse on atomic theory. At the same year Malus discovered polarized light. Wollaston related it to tetrahedron, but noted that *"It is perhaps too much to hope that the geometrical arrangement of primary particles will ever be perfectly known"*. In 1811 Dalton had a set of models of atoms and simple diatomic molecules constructed to help illustrate his ideas. In 1815 Biot observed several organic compounds that enable light polarization and realized that the rotation of light was due to a property of the individual molecule. In 1848 Pasteur found that crystals can be separated into two types, and in solution they rotated the plane of polarized light equally, but in opposite directions. This discovery could not be explained at that time due to lack of a proper model. The next indication of actual model construction was by Kekule in 1867, who proposed the tetrahedral structure of carbon bonds. In 1874 Van't Hoff used models- tetrahedra joined at the apex, sides or faces to describe the optical isomers of tartaric acid, which raised widespread objection. Sachse was one of the few chemists who around 1890 used molecules to make predictions, and predicted the 'boat' and 'chair' forms of cyclohexane. During 1900-1920 the use of ball-and-stick models became more widespread. In 1934 Stuart developed space-filling models that gave precise indications of the van der Waals radii of the atoms in a molecule. These were preferred over the earlier type, and opened the 'golden age' of molecular models. In 1947 Pitzer computed the energy barrier to carbon-carbon bond in butane. Later, Pitzer and Hazel, who won Nobel Prize in chemistry, demonstrated the axial and equatorial chair form of cyclohexane ring. Space filling models were considered an indispensable tool for organic chemists during the next 30 years and enabled the prediction of structural conformations, strereochemistry, reactivity and physical properties. Most notable was the double helix structure of DNA proposed by Watson and Creek in 1953, who later won Nobel Prize in chemistry.

Models in science and science education

Modeling and simulation are used in research and education to describe, explain and explore phenomena, processes and abstract ideas. Scientists, engineers and science educators use models to concretize, simplify and clarify abstract concepts, as well as to develop and explain theories, phenomena and rules. A model is considered useful if it is simpler than the natural object that it represents. An important value of models in science and science education is their contribution to visualization of complex ideas, processes and systems. A virtue of a good model is that it stimulates its creators and viewers to pose questions that take us beyond the original phenomenon to formulate hypotheses that can be examined experimentally[19,20]. Experimentation, however, is rarely presented as a way of developing, interpreting or evaluating explanatory models for the investigated phenomenon[21]. Ben-Zvi and Genut (1998) [22] recommended teaching high school students about interconnections of history and philosophy of science on one hand and the usefulness and limitations of scientific models, such as the Periodic Table, on the other hand. Gilbert and Boulter (1998) [23] distinguish between target systems, mental models, expressed models, consensus models and teaching models. Other researchers underscored the need for models as enablers of students' mental transformation from two-dimensional to three dimensional representations[24-26]. One of the problems that arise while using concrete models is that insufficient emphasis is placed on the fact that models are theory-based simulations of reality. The theory of molecular structure is a kind of intellectual model[27]. Harrison and Treagust (1996) [28] claimed that the use of term "model" is a source of considerable semantic variation for science students and teachers. Models are often oversimplified and therefore cannot tell humans all they may wish to know about the real physical system that is being modeled. Teachers and students should, therefore, be made aware of the fact that models, employed in a variety of research, study and design contexts, are not complete representations of the realities they are supposed to represent[29]. Applied to chemistry, physical ball and stick models derived from polystyrene spheres and plastic straws are not merely enlargements of the molecules they are intended to represent. These are analogue models that are used to explain new and abstract concepts. Some of the properties are similar to aspects of the target they are representing. For example, the relative diameter of the spheres represents the size of the different atoms. Other aspects, however, are not reflected in the model. For example, in a ball-and-stick model type, all sticks (straws) are of equal length, while "real" molecular bond lengths are not. Other analog models focus on different properties of the molecule, thereby creating multiple ways of representing the same molecule. Teachers frequently use just one type of model, limiting students' experience with models and causing their model perceptions to be partially or completely inadequate.

Computerized molecular modelling

The use of concrete molecular models (made of plastic, wood and/or metal) to illustrate phenomena in chemistry teaching has been widespread for a relatively long time[30]. The choice of model type has an impact on the image students create concerning the ways in which particles are shaped and how they function in the "real" world from a scientific viewpoint. Simulating different model types quickly and efficiently is achieved in a computerized environment, of which theoretical chemists, experimentalists and educators are taking advantage. Information technology helps relieving present-day researchers and students from the laborious task of data collection and enables them to engage in creative thinking and problem solving. Nakhleh and Krajcik (1994) [31] investigated how different levels of information presented by various technologies affect secondary students' understanding of acid, base and pH concepts. They found that students using microcomputer-based laboratories exhibited a positive shift in their concept map scores, indicating greater differentiation and integration of their knowledge. The development of computerized molecular modeling (CMM) made traditional models less favorable in the late 1960's. Not only are computers capable of drawing and manipulating molecules in three dimensions. They are also powerful tools for predicting molecular spatial structure through energy minimization calculations based on quantum mechanics. These capabilities have opened the way for advanced research in chemistry, resulting, among other things, winning Nobel Prize in chemistry (1998). Among the advantages of using information technology in science education are the options of providing for individual learning, simulation, graphics, and the demonstration of models of the micro and macro world[32]. Computer aided instruction enables students to solve a variety of problems while carrying out their own research at their own pace. The use of computerized models places more emphasis on the creation of mental models by students and their use to make prediction[23]. Students need more experience with models as intellectual tools that provide contrasting conceptual views of phenomena, and more discussion of the roles of models in the service of scientific inquiry. Raghavan & Glaser (1995) [33] recommend that science educators become less concerned with the presentation of facts and concentrate on showing the centrality of models in research and education. However, most educators use a limited number of static models, and do not emphasize the way in which models are created, their essential role in science learning, or their advantages and limitations. Williamson and Abraham (1995) [34] studied the effect of computer animations on college student mental models of chemical phenomena. Animations were used in two treatment situations: as a supplement in large group lectures and as both the lecture supplement and an assigned individual activity. Both treatments increased the students' understanding. They attributed the improvement to the superior formation of dynamic mental models of chemical processes that were made possible by the computer animation.



(a)

(b)

(c)

Figure 1 (a) Hand-Made primitive cubic unit cell; (b) Hand-Made body centered cubic unit cell; (c) Hand-Madeface centered cubic unit cell.

Conclusion

Interpretation of symbols, as well as understanding the particulate nature of matter and spatial structures are essential skills students need for solving problems in organic chemistry. However, model perception and understanding the spatial structure of organic molecules has been a source of difficulty for many chemistry students. A computerized molecular modeling (CMM)-based collaborative learning environment has been shown to be an effective means to overcome certain learning difficulties in chemistry.

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