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Curriculum Matters

MOLECULAR MODEL AND ITS SIMPLIFICATION IN TEACHING STEREOISOMERISM AT UNDERGRADUATE LEVEL

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Abstract. The role of molecular models in teaching chemistry is well-known. It is widely used in explaining the shape of molecules. Several authors have reported the difficulty in teaching stereochemistry/chirality. Some researchers have pleaded that the students face difficulty in solving stereochemistry problems because of poor visualization of three-dimensional structure of molecules. The present paper describes herewith the use of simple and inexpensive ball-stick molecular models in teaching stereoisomerism (conformation, configuration, and chirality in allenes) of organic molecules at undergraduate introductory organic chemistry course. It specially describes the use of simplified molecular models in determining the configuration (*R* or *S*) of the molecule.

Keywords: chemistry-teaching/learning; molecular-models; conformation; configuration; chirality

1. Introduction

The molecular models play a vital role in teaching science in general and chemistry in particular. The advantages of using molecular models in chemistry teaching are documented. According to Gilbert *et al*., the forms of teaching models that can also be considered to be scientific models include different representations of molecules – two-dimensional drawings, ball and stick models, space-filling models and computer simulations (Gilbert et al. 1998). In teaching at high school level chemistry, the molecular models can be used in a constructive manner to challenge students' internal knowledge schemes (Yager 1991). The use of teaching models in the classroom can encourage discussion and the expression of explanations that encourages students to evaluate and assess the reasoning behind their thinking (Raghavan et al. 1995). Boulter has reported that the importance of student discourse when using models constructively emphasizes the social aspect of learning (Gilbert et al. 2000). In a survey conducted by Mahajan and Singh on the factors affecting performance of year 1 students in organic chemistry, over two-third of the instructor from the SADC (South African Development Community) region had strong perception that the use of molecular models led to improved performance of students (Mahajan et al. 2005).

In the chemistry text books, the molecular structures are described in two dimensions using line formula (stick structures), space-filling models, and Fischer- projections. In learning organic chemistry, students often feel difficulty in visualizing the molecules in three dimensions (Copolo et al. 1995). A sound understanding of the molecular structure in three dimension is of utmost importance in understanding the mechanism of organic reactions and their stereochemical outcome.

Isomerism is defined as the difference in structures of molecules having identical molecular formula. The molecules with same molecular formula but different structures are called isomers. The constitutional/structural isomers are having different connectivity of atoms and hence they are easy to teach and students learn also easily. The geometrical isomers having same connectivity of atoms but different spatial arrangements that is challenging to students because of their limited ability to visualize the three-dimensional molecule in their mind (Wu et al. 2004; Kozma et al. 2000). The use of molecular models was devised in a workshop aimed at first year university undergraduate students to explain the concepts of stereochemistry (Baker et al. 1998). Obumnenye and Ahiakwo have reported improved performance of students in naming organic compounds by using stereochemical model (Obumnenye et al. 2013).

Chirality is among the trickiest concept to explain in organic chemistry. I have been observing from last several years that students of introductory organic chemistry course (year 2 of four-years' undergraduate program) struggle in understanding the concept of conformation, determination of *R*- and *S*-configuration and, the enantiomerism in molecule without any chiral carbon especially allenes. However, the use of simple ball-stick model makes it very easy to teach these concepts in class. The paper describes herein easy use of this model in explaining conformation, determination of *R*- and *S*-configuration and, the enantiomerism in organic molecules.

2. Application of Molecular Models in Teaching Stereoisomerism

2.1. Application of Molecular Models in Teaching Conformation

Conformational isomers or rotamers in alkanes are due to free-rotation around C-C single bond while that in cycloalkanes are due to ring-flip. A teacher cannot perform both these operations on a lecture board. As a result, the students get puzzled when they are taught that one methyl (CH_3) of the ethane molecule moves freely around other methyl group, or the cyclohexane ring is not planar but chair-shaped and all the hydrogen atoms in the cyclohexane ring are not equivalent; six of them are occupying equatorial positions and six axials. Using a ball-stick model for showing the free-rotation in alkanes and flipping of the ring make the task much easier for the teachers and learners. The students get amazed when they see methyl group moving freely around each other in ethane giving staggered and eclipsed conformations or six hydrogen atoms going above and below the plane of the ring (axial) and six hydrogen atoms occupying equatorial position on the cyclohexane ring. The Newman projection of the staggered and eclipsed conformations of ethane, ball-stick model of staggered conformation of ethane, chair conformation of ethane and its ball-stick model are shown in Figure 1 – 4.

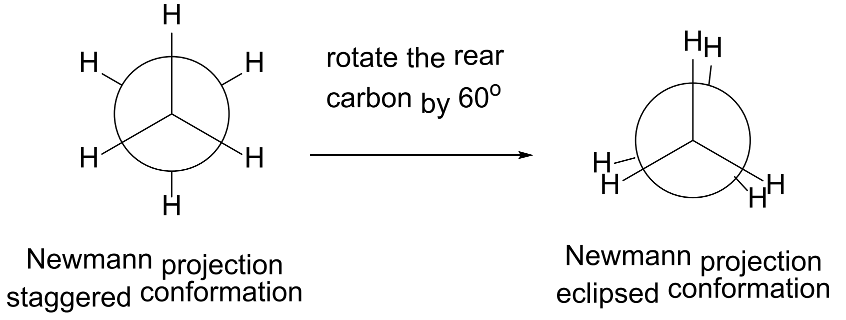

Figure 1. Newman projections of staggered and eclipsed conformations of ethane

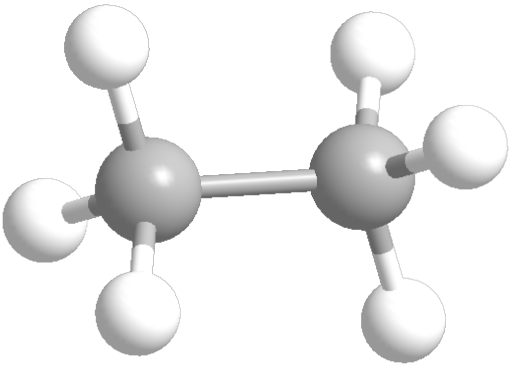

Figure 2. Ball-stick model of staggered conformation of ethane

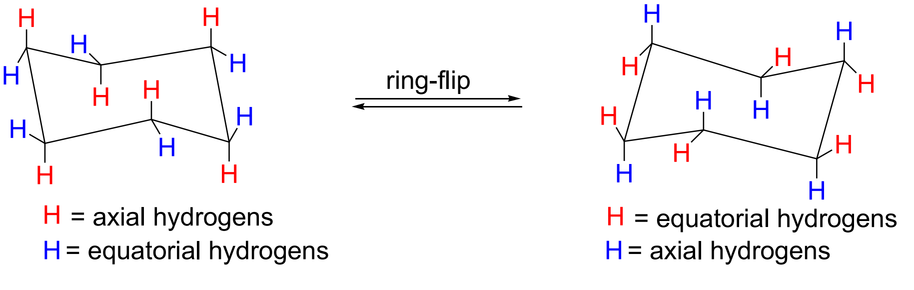

Figure 3. Chair conformation of cyclohexane

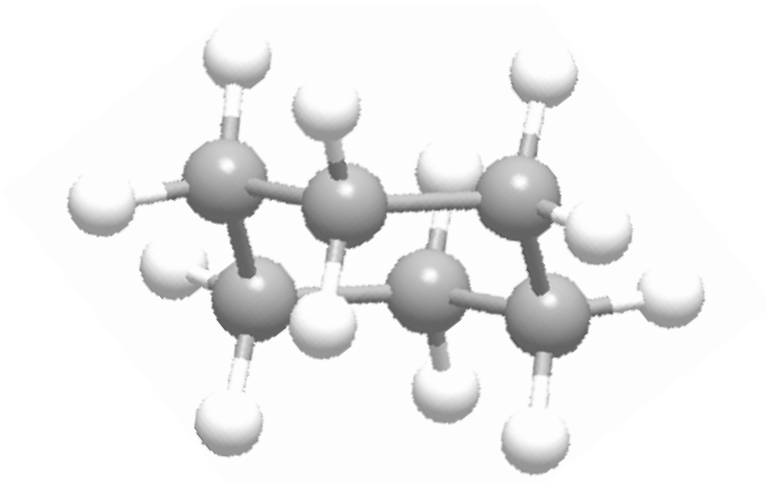

Figure 4. Ball-stick model of chair conformation of cyclohexane

2.2. Application of Molecular Models in Teaching Determination of R- and S-Configurations

The different textbooks and different teachers even though using the same convention of drawing can draw the structure of a particular molecule in different ways. Simply exchanging the position of the two groups make students unable to view the structure in three-dimension and decide whether it is (*R*) or (*S*) configuration. It is therefore always advisable to students to carry molecular model with them I the class. Many students avoid carrying models thinking that it is difficult to construct the molecular models of complex molecules in class-time. Of course, making model of complex molecules are time consuming but here one has to see the objective of making the model. The only objective of the model in determining the configuration is to see the order of the high to low priority groups (clockwise or anticlockwise) in the molecular model. For this purpose, there is no need to make the complete model of the molecule. One need to carry only four sticks and five different color balls. The priority of the atom/groups can be decided on the paper; to do this one does not need a three-dimensional view. After deciding the priority of all four groups, four balls of different colors can be taken, and they can be arbitrarily assigned priority 1 – 4 as shown in the Figure 5. Now one can make model of the structure given using just a carbon ball, four sticks, and four ball. The different color balls have to be attached exactly on the position where shown in structure on the piece of the paper. The model can be rotated freely to see whether the groups 1 – 3 are clockwise or anticlockwise. It can be clearly seen from the model of (*S*)-2-chlorobutane that the highest to lowest priority groups are in anticlockwise manner. For (*R*)-2-chlorobutane, it is difficult to visualize whether it is clockwise or anticlockwise. If one has model in hand, it can be easily moved to arrange the groups (1-3) in clockwise or anticlockwise manner as shown in Figure 5. Also, the position of two balls can be exchanged and shown that exchanging the position of two groups gives enantiomer.

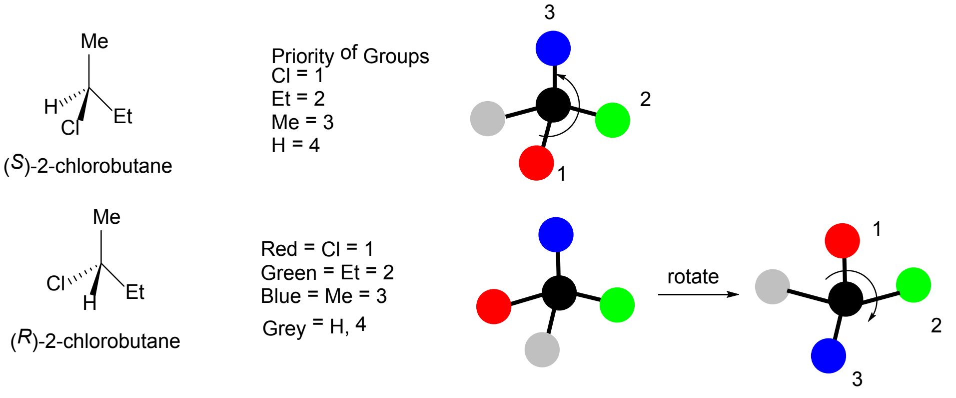

Figure 5. Enantiomers of 2-chlorobutane

2.3. Application of Molecular Models in Teaching Chirality in Allenes

Teaching enantiomerism in allenes is like hitting head on the wall. Allenes are not planar molecules. Unless one has a model, it is extremely difficult to convince the students that half of the molecule will have a mirror image and half will look identical in the mirror image. Using simple ball-stick model (Figure 6), one can show to the students how the mirror image of a particular allene will look like. According to Figure 6, the H and Cl atoms in the upper half of the molecule are in the plane of the paper and hence produce mirror image. The H and Cl atoms in the lower half of the molecule are perpendicular to the plane of the paper, and hence they will look identical in mirror. The overall mirror image will be thus non-superimposable and hence enantiomer.

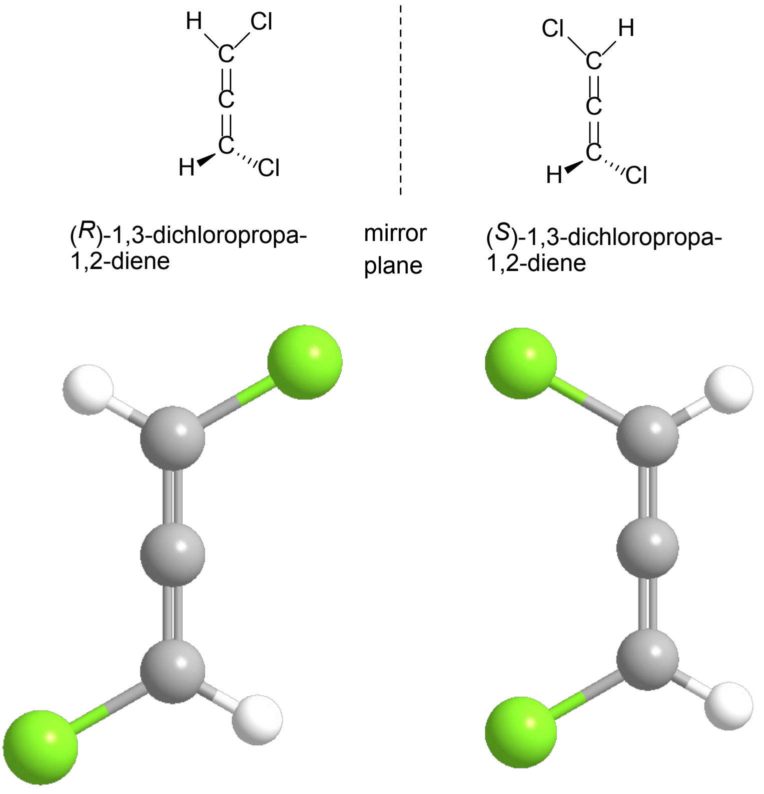

Figure 6. Enantiomers of 1,3-dichloropropa-1,2-diene

Conclusion

The use of simple non-expensive ball-stick molecular models can make teaching and learning of stereoisomerism easy and simple. These simple models can be used for effective teaching of conformation, determination of (*R*)- and (*S*)-configurations, and enantiomerism in allenes. There is no need to make the complete model of the molecules; instead, simplified models can be made to understand the points in question.

REFERENCES

Gilbert, J.K., & Boulter, C.J., 1998. Learning science through models and modelling. In *B. J. Fraser & K. G. Tobin (Eds.), International Handbook of Science Education,* 53 – 66. Dordrecht, The Netherlands: Kluwer Academic Publishers.

Yager, R.E., 1991. The constructivist learning model: Towards real reform in science education. *Sci. Teach.* **58**, 52.
Raghavan, K., Glaser, R., 1995. Model-based analysis and reasoning in science: The mars curriculum. *Sci. Educ.* **79**, 37.
Gilbert, J.K., Boulter, C.J., (Eds.)., 2000. *Developing models in science education*. Dordrecht, The Netherlands/Boston/London: Kluwer Academic Publishers.
Mahajan, D.S., Singh, G.S., 2005. University students' performance in organic chemistry at undergraduate level: Perception of instructors from universities in SADC region. *Khimiya* **4**, 25.
Copolo, C.F., Hounshell, P.B., 1995. Using three-dimensional models to teach molecular structures in high school chemistry. *J. Sci. Educ. Technol.* **4**, 295.
Wu, H. K., Shah, P., 2004. Exploring visuospatial thinking in chemistry learning. *Sci. Educ.* **88**, 465.
Kozma, R., Chin, E., Russell, J., Marx, N., 2000. The roles of representations and tools in the chemistry laboratory and their implications for chemistry learning, *J. Lear. Sci.* **9**, 105.
Baker, R.W., George, A.V., Harding, M.M., 1998. Models and molecules: A workshop on sterioisomers, *J. Chem. Educ.* **75**, 853.
Obumnenye, N., Ahiakwo, M.J., 2013. Using stereochemistry models in teaching organic compounds nomenclature: effect on senior secondary students' performance in rivers state of Nigeria. *African J. Sci. Educ*. **3**, 91.

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