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DRAWING CHAIR CONFORMATIONS IN LEARNING PHARMACEUTICAL CHEMISTRY

a chapter by

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Abstract

A series of six-hour lectures in introducing organic chemistry to pharmacy learners were designed with practical hours on how to draw chair conformations to represent a three-dimensional representation of closed carbon atoms ring or cyclic structures. The lesson was provided during both face-to-face sessions, and virtual classes when the pandemic semester begun. The students were taught to draw the two-dimensional views of the molecule during their foundation study, prior to the pharmacy undergraduate program. However, when it comes to three-dimensional illustrations, the students should be able to imagine the upper and lower part of a cyclohexane plane, as they would sit on a chair. Such imaginations are important since the carbon atoms are not positionally equivalent. For the purpose of teaching and learning, two students' batches were invited to submit their drawings. Majority of them showed their efforts, as part of the lecture participation. It was found that most corrections would involve the imaginary parallel axis, to draw both equatorial and axial bonding of the cyclohexane, a six-membered hydrocarbon structure. In summary, this drawing exercise could serve the knowledge of the molecular conformations, as they would later observe in chemical structures having higher atomic weight, such as the pharmaceutically important steroidal molecules, with fused five- and six-membered rings.

Keywords: *chair, chemical, drawing, molecule, pharmacy*

Introduction

Science stream students were taught to draw the two-dimensional (2D) views of the molecules during their foundation studies. The ability to illustrate chemicals are important, to assess the students on their knowledge of the bonding, especially involving the organic compounds or the hydrocarbons. The fact that carbon atoms can only hold four single bonds, would guide the students on how to ensure the natural stability of the atomic mixtures. Furthermore, carbon atoms can be linked in straight, branched and ring forms to build various compounds, with medicinally important properties, as manifested in drug molecules, such as the steroids (Sarker et al. 2007; Barlow, 2014). Once the students enrol into the pharmacy program, they are taught to draw both two- and three-dimensional (3D) structures. However, when it comes to 3D illustrations, the students should be able to imagine the upper and lower part of a plane, as they would sit on a chair. Such imaginations are important since the atoms are not equivalent, in terms of their position, in space. This is the case of learning cyclic molecules, for example, the cyclohexane (Figure 1) and its derivatives (Dewick, 2006). This saturated molecule has six carbon (C) atoms, each of them has two hydrogens. It has a total of twelve hydrogens (H), hence, the formular molecule is C6H12 (Figure 1a). The bond line formula of this molecule is shaped like a hexagon and a chair, respectively in 2D and 3D. It would then, provide two types of hydrogen atoms, either in axial or equatorial positions. Therefore, there is a total of six axial hydrogens; three axial hydrogens are above and another three axial hydrogens are pointing below (Gareth, 1996). In the meantime, there are six equatorial hydrogens, directing away from the chair (Figure 1b). A series of six-hour lectures in introducing organic chemistry

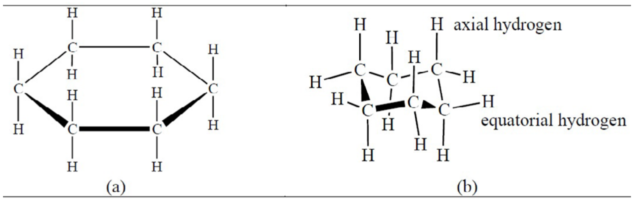

Figure 1: The structural drawing for cyclohexane in 2D (a) as a flat hexagon, having six straight, equivalent sides and six internal angles. There are six carbon (C) atoms arranged in a closed ring, while the hydrogen (H) atoms are linked above and below the hexagon. Meanwhile in (b), cyclohexane is shown in a non-planar, 3D chair conformation. Some C-C bonds are bold to show that they are closer to the viewer.

to pharmacy learners was planned with practical hours on how to draw chair conformations to represent a three-dimensional representation of closed carbon atoms ring or cyclic structures, as depicted in cyclohexane molecule (Figure 1). These lessons were provided during both face-to-face sessions, and virtual classes when the pandemic semester begun. Examples of the drawing will be shown, here. It is hypothesised that the students could understand the concept of the chair conformer, should their sculptural drawings of the cyclohexane, in a chair form, are accurate.

Methodology

Two students' batches (September intakes) were invited to individually submit one drawing of cyclohexane in its chair conformation. This call was made at the end of the first PHC414 Fundamentals of Pharmaceutical Organic Chemistry lecture, in the first week of both semesters. There were 174 and 176 students, sequentially from 2020 and 2021 enrolments. The drawings were forwarded by email as pictorial or multimedia messages to the lecturer-in-charge.

Result & Discussion

Majority of the students (90% of both cohorts) showed their efforts, as part of the virtual lecture participation in Week 1 and 2 of the semester. It was found that most reminders and corrections involved the imaginary axis, passing through the centre of the ring (Figure 2), parallel to the axial hydrogens, in order to draw both axial and equatorial hydrogen bonding of the cyclohexane ring.

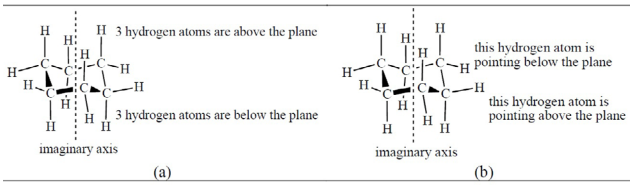

Figure 2: The structural drawing for cyclohexane (a) showing the imaginary axis to the students, as a guide to sketch six carbon-hydrogen (C-H) bonding, three above and another three below the plane. Meanwhile in (b), another six hydrogens are drawn in equatorial positions, with alternate orientations, pointing above and below the plane.

Some representational translation from 2D structures of cyclohexane to its chair conformations, with common student errors, were also observed, as commented by Mistry et al. (2020). Among the feedbacks that were relayed to the students include the following;

(a) completing the missing carbon-hydrogen (C-H) bonds (Figure 3a),

(b) aligning the bonds for building the plane inside the chair conformer (Figure 3b),

(c) drawing equal C-H and carbon-carbon (C-C) bond lengths (Figure 4a), since they are equivalent C-C and C-H, respectively.

(d) making connections, since there is a standard drawing method to display chemical bonds. The front bonding line is connected, meanwhile, the back line is disconnected. This is to distinguish different atomic bonds to the viewer (Figure 4b).

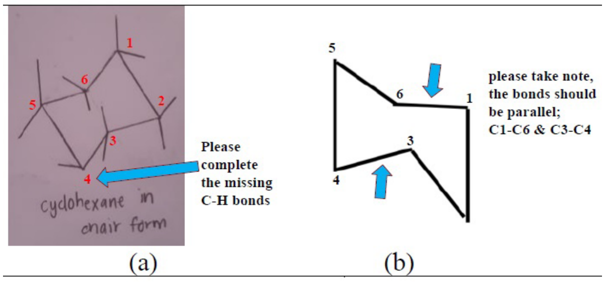

Figure 3: (a) An example of a student's incomplete drawing for cyclohexane, and (b) showing the unaligned bond, to correct the plane in the chair.

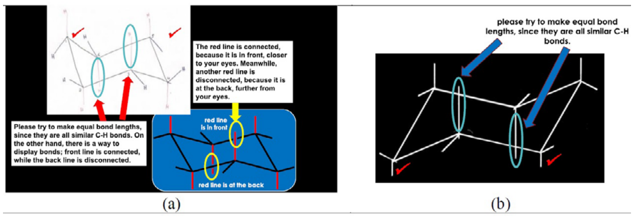

Figure 4: (a) Some examples of student's drawing for cyclohexane, with errors and (b) showing the standard way to make chemical connections or bonds, either closer or further to the viewer.

The students' imagination were also tested while visualising the mirror images of their chairs (Figure 5a). This is because the chair owns its mirror image, thus, it is not superimposable with one another. Here, the concept of flipped or converted chair could be introduced, since cyclohexane would exist in both conformations or configurations. In another word, there is a 50% chance to find this molecule in one shape or chair, and other 50% chance in its mirror image. When a chair conformation "flips" to give the other chair conformation, the axial hydrogens would become equatorial, and the equatorial hydrogens would become axial (Figure 5a). In one trial, a student's carbon ring skeleton still looks like the original chair, not its reflection (Figure 5b). The student was reminded to keep on practicing "flipping" the cyclohexane chairs, after the lectures.

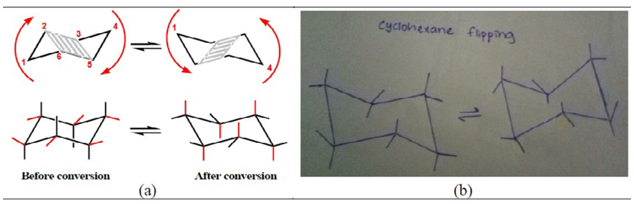

Figure 5: (a) An example to draw the chair, plus its mirror image. While, in (b) a student's converted chair was not the mirror image of the original cyclohexane.

Other cyclic compounds with lower number of carbon (C), for example, the cyclopropane, has three C atoms, each of them has two hydrogens, and it is in a flat, closed-ring form, or just like a triangle (McIntosh, 2022). In the case of a cyclobutane with four C atoms, it could occur as a non-flat molecule, with internal C-C-C angle as 88_o. This hydrocarbon can also adopt the butterfly shape, having equatorial and axial hydrogens (Parsons, 2014). Therefore, a lecturer's common advice to students is to use molecular model (Prentice Hall Molecular Model Set For Organic Chemistry, 1983) to help them understand the geometry of cyclic compound (Figure 6) and other organic chemicals.

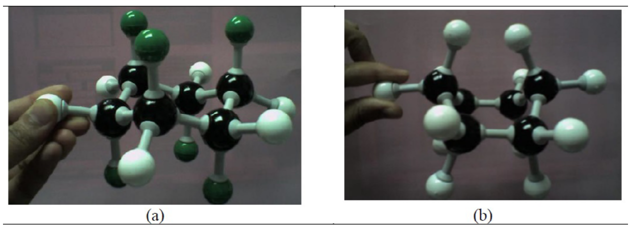

Figure 6: (a) A cyclohexane model is shown as the most stable conformation in its chair form and is held at one of the equatorial hydrogens, as demonstrated in the practical class.
(b) The cyclohexane with a boat shape is displayed, as one of the non-stabilised conformers.

One of the difficult skills for students to develop is the chemical visualization from 2D representations, as commented earlier (Dauphinee et al. 1983). This is particularly evident in the drawings of cyclohexane rings (Figure 3). Furthermore, the ball and stick modelling kit would not be the main choice in pandemic semesters. During the movement limitation, it is fortunate that most students were able to complete their course task, despite the lacking of face-to-face coaching and interactions (Azman et al. 2022). Lecturers and educational researchers continuously ponder on how to overcome the difficulties and how to help the students understand the drawing topic better. Therefore, the use of devices, online computational technology such as MolView (an open-source web-application) and mobile game (Winter et al. 2016), could facilitate students' comprehension of concepts in configurational chemistry. Hussaini and Secka (2021) have described step-by-step instructions that use cyclohexane projections to help the students draw the lowest energy conformers of the molecule. In an advanced effort, 3D animations for chemistry courses were developed and became the basis for the 3D augmented reality tool. According to students' feedback, technologies could help students overcome barriers, presented by traditional ball and stick modelling methods (Abdinejad et al. 2020).

Conclusion

The drawing exercise could serve the basic knowledge of the molecular conformations during the foundation year of pharmacy students. Towards their practical years, the students would be able to observe the significance of molecular geometry involving chemicals with a much higher atomic weights and drug molecules, such as the pharmaceutically important steroids, having fused five- and six-membered carbon rings.

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