doi:10.2533/chimia.2021.54 Chimia 75 (2021) 54–57

Structure Drawing at the Heart of Teaching Chemistry

Ágnes Peragovics* and Erika Biró

Abstract: Chemistry is all about structures. There are myriads of structural representations that are required for the students to become familiar with when learning chemistry. Structural formula, skeletal formula, Lewis and resonance structures, three-dimensional representations are just a few examples of the drawing styles that should be readily interpreted by a chemistry student. In order to gain the necessary knowledge to understand and manipulate chemical structures, students must extensively solve problems with structural illustrations and practice drawing chemical structures themselves. Here we present Zosimos, an online chemistry educational tool with comprehensive structure-drawing capabilities that allows chemistry teachers to create real chemistry quizzes, share them with their students and get immediate feedback on their learning progress. 5th grade students at Kantonsschule Zug have been learning chemistry with Zosimos since September 2019 and this article also shares insights on how to implement this learning tool in a real classroom setting.

Keywords: Chemistry education · Online learning · Organic chemistry · Structure drawing

Ágnes Peragovics graduated from the Budapest University of Technology and Economics as a chemical engineer. After finishing her graduate studies, she completed her PhD in the field of pharmaceutical research. She first joined ChemAxon in 2013 and worked as an Application Scientist on several products. She also worked as a Sessional Lecturer at the University of British Columbia in Vancouver where she taught physical chemistry to international students. Having experience from the teacher-side, she rejoined ChemAxon and the Zosimos team as an Application Scientist in 2019.

In love with computer science, ***Erika Biró*** first got involved with chemistry computational science in 1998, after graduating with a software engineering and mathematics degree at Eötvös Loránd University, Budapest. As a research assistant for 5 years at ICAMS, School of Chemistry, University of Leeds, she took part in the development of a system called SPROUT that can assist in several stages of the structure-based rational drug design process. In 2005 she joined ChemAxon and went on developing Marvin, the drawing and editor tool. ChemAxon decided two years ago to build a new platform to support chemistry education where, since then, she is an active contributor as a product manager.

1. Introduction

Chemistry relies heavily on structural representations. Fig. 1 shows some example representations that are commonly used to depict chemical structures such as skeletal formulas, three-dimensional structures, and Lewis structures. However, interpreting, manipulating, and switching between the numerous structural representations is a complicated task for many students.[1] To be able to predict the reactions and properties of molecules, students must practice chemistry little by little every week, and practice solving molecular representation and reaction drawing problems.

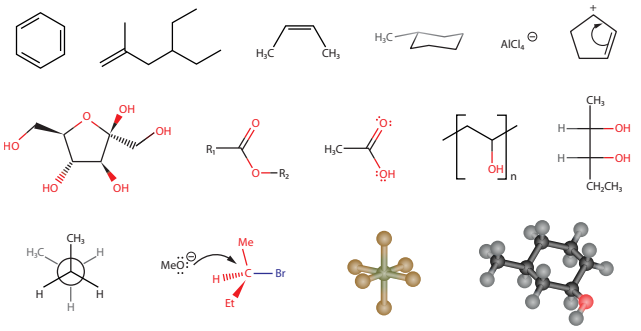

Fig. 1. Some examples of the different structural representations used in chemistry.

Consequently, any digital learning tool used to support chemistry teaching is desired to have chemistry drawing capabilities.[2,3] This functionality is essential for teachers to create meaningful chemistry exercises and also vital for the students to practice drawing chemical structures. This year has posed many challenges to educators worldwide because of the coronavirus global pandemic[4] and resulted in a growing need for a chemistry learning platform that enables the students to practice and write assessments from home, while still showing off their compound drawing and interpretation skills.[5]

Here we would like to introduce Zosimos, an online chemistry educational tool that allows chemistry students to independently practice and learn a wide range of structural representations in a quiz format, and get immediate feedback on their progress. Zosimos is built on ChemAxon's JChem[6] and Chemicalize technology[7] and integrates the chemical drawing tool Marvin JS.[8] This new educational tool is available in the form of a web application at *https://zosimos.io* for computers, tablets, and smartphones. Zosimos

*Correspondence: Dr. Á. Peragovics, E-mail: aperagovics@chemaxon.com
ChemAxon, Záhony utca 7., Building HX, 1031 Budapest, Hungary

is supported on Google Chrome, Mozilla Firefox, Apple Safari and Microsoft Edge.

2. Supporting Chemistry Education

ChemAxon's chemical drawing tool, Marvin JS is seamlessly integrated into Zosimos (Fig. 2). Molecule images may be added easily when creating chemistry quizzes and teachers can use the molecule editor without any restrictions to illustrate their exercises. Drawn compounds may range from small molecules to large complexes or even to reactions. There are also different visualization settings available to choose from that allows the teacher to select their preferred drawing style (*e.g.* skeletal or structural) and whether they would like to use 2D or 3D representations.

Zosimos offers three different exercise types that can be used when creating chemistry quizzes. In the following we will review the different exercise types that are currently available in Zosimos with special attention to the structure drawing options that are built-in for each exercise.

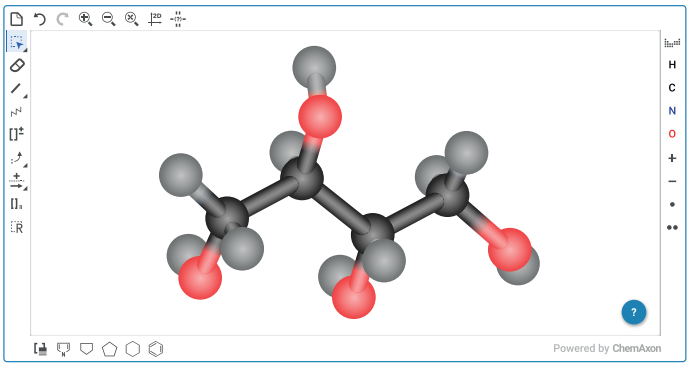

Fig. 2. Chemistry drawing in Zosimos is supported by the chemical editor Marvin JS.

2.1 *Text Answer*

This is a non-drawing exercise type for students which requires them to enter a text when completing the exercise. However, with the help of the chemical editor, these exercises can be widely illustrated with structural content such as shown in Fig. 3.

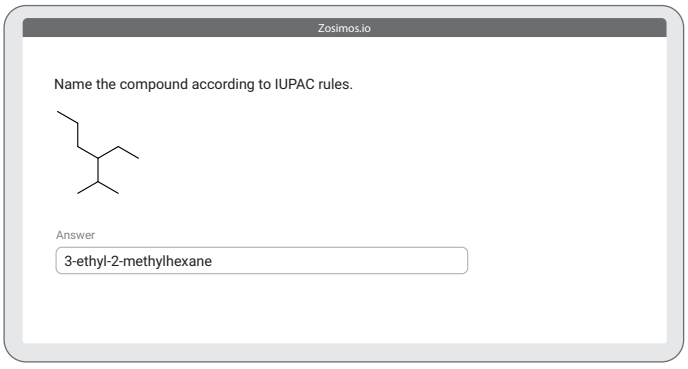

Fig. 3. A nomenclature exercise using text answer.

This type of exercise is commonly used in nomenclature problems, for example, or when checking the understanding of chemical concepts. It also supports the creation of fill-in-the-blanks type questions. Teachers may also define multiple alternative text answers if more than one correct answer satisfies their exercise. If the student's answer matches the text that has been provided by the teacher, the student gets a certain score for the exercise that was set by the teacher.

2.2 *Multiple Choice*

The commonly used multiple choice exercise type is also available in Zosimos, including single-answer and multiple-answer variants. It is also equipped with chemical drawing possibilities: teachers may add chemical drawings as options in a multiple choice exercise and they can select their preferred drawing style. This type of exercise may be used, for example, when asking about properties of compounds (see Fig. 4, for example) or checking for correct interpretation of structural features in molecules.

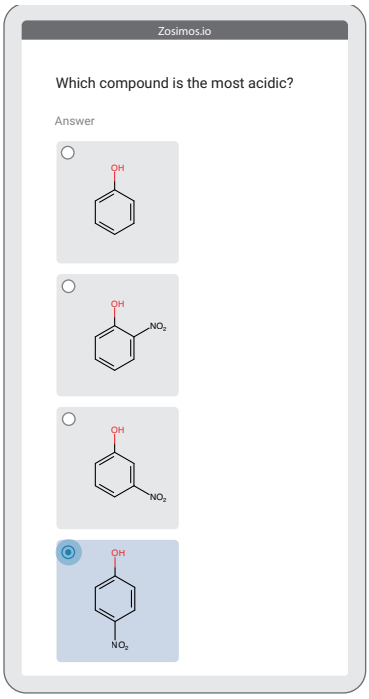

Fig. 4. Students can select the correct answer(s) from a set of structures in the multiple choice exercise.

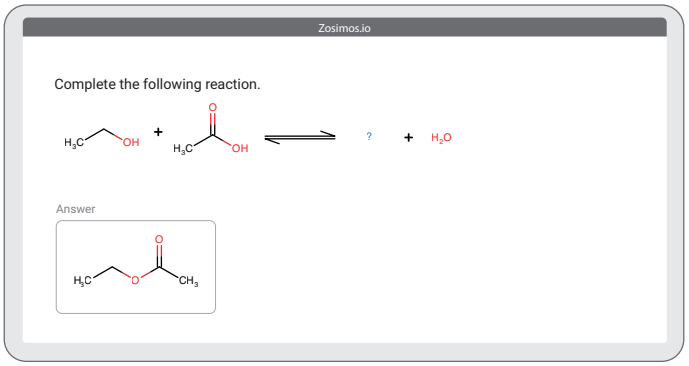

Fig. 5. Students draw molecules when providing structure answers.

2.3 *Structure Answer*

Chemical structure drawing may also be expected from students as correct answers (Fig. 5). We support the drawing of Lewis structures, ions, resonance structures and several stereochemical representations such as dash-wedge structures or *E*/*Z* isomers. This exercise type is often used to request drawing isomers, predict the product of reactions, draw molecules from IUPAC names or switch between structural representations.

When students are practicing with this exercise type, they will be able to draw the requested compound from scratch and their structure will be compared to the correct structure provided by the instructor. If the student's structure matches that of the

instructor, the student receives the points for that exercise. The checking algorithm behind this exercise type is equipped with chemical intelligence: it checks for atom types, the bond order and the connectivity of the atoms, lone pairs and charges. It is also able to check for polymer structures, resonance structures, polyatomic ions, R-group representations, and recognizes reaction features such as + signs and the different arrow types. Curved arrows may also be evaluated in reactions when asking questions about reaction mechanisms. We also recognize several different types of stereochemical representations such as wedge and dash projections, *E*/*Z* stereoisomers.

In certain exercises, the instructors may want to aid the students' work by providing a starter structure to work on. Zosimos uses templates of predefined molecules that will show up for the students upon exercise completion. Students can modify these template compounds when answering the questions (Fig. 6).

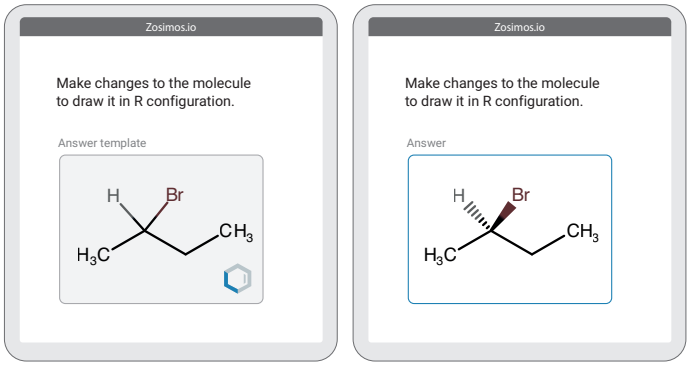

Fig. 6. Students are presented with pre-drawn structures and are asked to modify them.

3. How to Use Zosimos with a Class

Students can be invited by instructors to join a class in Zosimos. The chemistry quizzes created by the instructor may be used in the following two different ways in a class.

3.1 *Practice Quizzes*

The chemistry quizzes can be shared in a practice mode. In this case, the students can complete a specific quiz as many times as they want for their own practice. Students may also try to answer a specific question several times if the teacher allows more than one attempt. The instructor can view their results in the class, thus they can continuously monitor the students' progress. This type of usage supports the recognition that chemistry is a difficult subject and requires frequent practice from the learner to master the new concepts.

3.2 *Assessments*

Another way of using chemistry quizzes with a class is to make assessments. This is a more formal way of using the quizzes and enables the instructors to prepare homework, exams, assignments, and other types of tests for their students. Assessments can be accessed by the students within a limited time frame that is controlled by the instructor. In contrast to the practice mode, students can complete the quiz only once when doing an assessment. Once the assessment time is over, the instructor can review the students' results in Zosimos and download the assessment scores in a csv file.

4. Class Independent Usage

Zosimos may also be used without creating a specific class. The following two options are available in the tool for teachers and students alike to solve chemistry problems and practice molecular structures without the need of setting up or joining a class.

4.1 *Public Quizzes*

Zosimos offers a large number of quizzes that are immediately available after registration. These quizzes cover diverse chemistry topics and have been created by chemistry experts at ChemAxon and by our registered teachers who decided to share their learning material with the teacher community. The public quizzes may be used without any limitation with students or can serve as starting points for quiz creation. Thus, it is possible to cherry pick some of the exercises of a public quiz and develop personal content from these quizzes. Since our teachers are located around the world, the language of the quizzes varies. Currently we have English, French, German and Spanish chemistry quizzes, to mention just a few.

4.2 *Memory Game*

Zosimos also includes a Memory Game to support playful learning. Students can learn and review chemical structures by turning over cards and looking for matching structures. Amino acids may be matched by their names or compound classes can be reviewed by looking for functional groups.

5. Instructor Experiences and Student Perceptions

5.1 *General*

The Zosimos Early Adopter program provides teachers with early access to Zosimos. Members of the early adopter program play an important role in the product development process by sharing feedback on their Zosimos experience, contributing ideas and enhancement requests while having free access to all Zosimos functionalities for their classes. Urs Leisinger started using Zosimos as a participant of our Early Adopter program at Kantonsschule Zug (Kantonsschule Zug, Lüssiweg 24, CH-6302 Zug) in September 2019. Kantonsschule Zug is one of the high schools that was awarded the 'MINT-Label' by the Swiss Academy of Sciences. MINT stands for mathematics, informatics, natural sciences and technology. This prize is awarded to high schools that are particularly active in the field of science and technology.

In the following part, we summarize what has been experienced at Kantonsschule Zug in relation to the students' Zosimos practice. In order to gain more insights into their Zosimos usage, Urs Leisinger was asked to answer the following set of questions:

1. What are the high school chemistry topics that can be supported by Zosimos?
2. How old are the students you use Zosimos with?
3. How many students are using Zosimos?
4. What kind of activities do you prepare for the students in Zosimos?
5. How do they learn to use the drawing tool?
6. What do you see as the learning benefit of using Zosimos?
7. What do the students say about Zosimos? What kind of feedback did you get from them?
8. How does Zosimos help your teaching in the time of COVID-19?

The following part of the article was created based on his answers given in this mini interview.[9]

5.2 *High School Chemistry Topics*

5th grade students (around 40 to 60 students per year, age 17–18) at Kantonsschule Zug are frequently set obligatory and optional exercises in the practice mode of Zosimos to support their chemistry learning. According to Urs Leisinger's experience, Zosimos may support the learning of any part of the high school chemistry curriculum where drawing molecules is required. Some example topics have been collected here that were covered at Kantonsschule Zug:

a) Introduction to molecules

Students can be asked to practice drawing small molecules, mono-atomic ions and polyatomic ions. Students can also practice the octet rule with Zosimos to be able to draw correct structures.

b) Conjugated systems
c) Hydrogen bonding

Students can draw molecules with certain hydrogen bonding properties in exercises like this: "Draw a molecule that consists of 2 C atoms, 1 O atom and as many H atoms as needed and contains one donor residue and can maximally form three hydrogen bonds."

d) Acids and bases
e) Organic nomenclature

This topic will be exclusively supported in Zosimos this year with practice quizzes.

f) Organic reactions

5.3 *Learning Benefits*

Several learning benefits have been identified at Kantonsschule Zug related to using Zosimos regularly with the students: Firstly, Zosimos offers the opportunity that everyone can work on chemical structures at their own speed. Students never have to wait for corrections or feedback from the teacher, nevertheless they clearly know how they have performed. This can reduce waiting time and generate more learning time.

Secondly, using Zosimos also adds a gamification component to the students' practice. When providing short exercises to the students, they may get in a gaming mood. U.L. observed that a certain fraction of students solves the exercises several times because they would like to improve on completion speed and correctness. Additionally, even those students can be included in the Zosimos activity who otherwise have to fight high activation barriers when they are expected to solve problems on their own.

Lastly, Zosimos is optically attractive, has a modern look and is a modern digital tool. All of these factors can motivate students to study more intensively. However, it should also be noted that while Zosimos is a useful tool for practicing, it should not replace the elaboration and discussion of carefully chosen examples. Students must also draw in their documentation that is compiled in a way to give a maximal overview.

5.4 *Student Feedback*

Students like the immediate, clear and precise feedback they get when using Zosimos. They also like the fact that the teacher needs less time to correct exercises, therefore they have more resources to discuss problems related to their personal understanding of chemical theories. However, it should be noted that using Zosimos still requires a considerable time investment from the teacher's side especially in the exercise preparation process.

U.L. noticed that some students had some difficulties using Zosimos at the beginning. The chemistry they should practice is already demanding and they find the extra difficulties to learn to navigate a new platform sometimes overwhelming. To overcome this problem, students received plenty of hands-on tasks, where they learn through trial and error and by supporting each other. Zosimos is very intuitive, but for new users it is nevertheless quite complex. A lot of details have to be clear before the students can focus on the chemical part of the work.

5.5 *Instructor Notes*

From the instructor's point of view, it is very useful to have a look at the incorrect responses and review which part of the exercise the students were able to solve and what was problematic for them. When looking at their different attempts at solving an exercise, it is usually clear what causes their problem and it can be explained to them individually, without forcing the rest of the class to listen to the explanation. During the coronavirus lockdown, Zosimos proved to be extremely useful because of this easy tracking of the students' progress.

For homework, a small number of questions (3–8) proved to be effective, where each question deals with a different aspect. The number of attempts were usually set to three. Thus, if the students do not provide the right answer at the first attempt, they can try solving the exercise two more times. After three attempts it is better to give them the solution (and another exercise with similar challenges), otherwise the attention breaks off.

U.L. is also experienced in using Moodle to support his chemistry teaching. Compared to that learning platform, he especially likes Zosimos because of its user friendly and intuitive interfaces for students and teachers alike. Also, he greatly appreciates the autocorrection algorithm which takes into account fine chemical details such as the presence of lone pairs in a chemical structure.

5.6 *Future Plans*

The number of students using Zosimos will be extended at Kantonsschule Zug this year. Besides 5th graders, students learning chemistry at grades 3, 4, and 6 will also have a chance to practice chemistry in Zosimos. The reason behind this planned extension is twofold. On one hand, the instructor feels that Zosimos is now mature and versatile enough for wider usage. Also, the school has recently changed to a bring your own device scenario (BYOD), meaning that every student brings along their own computer to the school. Now that the computers are always available, the Zosimos exercises can easily be integrated into any learning setting.

6. Closing Remarks

Zosimos can be tried out at *https://zosimos.io*. After a short registration, teachers can start browsing the chemistry quizzes prepared by other instructors or start creating their own exercises. We offer Zosimos in two packages, Basic and Pro, with a 1-month free trial period of the Pro package.

Zosimos is under active development at ChemAxon so its chemistry capabilities are expected to grow further. Our plans include supporting exercises with multistep synthesis to extend our chemistry towards advanced organic chemistry. Also, we would like to offer more exercise types to further support the learning of general chemistry and inorganic chemistry.

Acknowledgements

We thank Urs Leisinger (Kantonsschule Zug) for his ongoing participation in the Zosimos Early Adopter program and for sharing his teaching experience with Zosimos in this article. We also would like to thank the Zosimos team at ChemAxon for their work on the product development.

Received: November 13, 2020

[1] N. Graulich, *Chem. Educ, Res. Pract.* **2015**, *16*, 9, https://doi.org/10.1039/C4RP00165F
[2] B. Jaun, C. Thilgen, *Chimia* **2018**, *72*, 48, https://doi.org/10.2533/chimia.2018.48
[3] C. I. C. Crucho, J. Avó, A. M. Diniz, M. J. S. Gomes, *J. Chem. Educ.* **2020**, *97*, 3211, https://doi.org/10.1021/acs.jchemed.0c00693
[4] N. Dietrich, K. Kentheswaran, A. Ahmadi, J. Teychené, Y. Bessière, S. Alfenore, S. Laborie, D. Bastoul, K. Loubière, C. Guigui, M. Sperandio, L. Barna, E. Paul, C. Cabassud, A. Liné, and G. Hébrard, *J. Chem. Educ.* **2020**, *97*, 2448, https://doi.org/10.1021/acs.jchemed.0c00717
[5] T. M. Clark, C. S. Callam, N. M. Paul, M. W. Stoltzfus, D. Turner, R. Spinney, *J. Chem. Educ.* **2020**, 97, 3413, https://doi.org/10.1021/acs.jchemed.0c00546
[6] https://chemaxon.com/products/jchem-engines
[7] https://chemicalize.com/welcome
[8] https://chemaxon.com/products/marvin-js
[9] U. Leisinger, personal communication, October 22, **2020**.