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TEACHING THE FUNDAMENTALS OF MOLECULAR SYMMETRY IN HIGH SCHOOL THROUGH THE USE OF THE INTERACTIVE ONLINE RESOURCE SYMOTTER

Abstract: Molecular symmetry is a fairly complex branch of chemistry that requires special teaching methods, including the integration of traditional approaches with modern visualisation and modelling technologies. The article discusses the possibilities and results of using the Symotter online resource for studying the fundamentals of molecular symmetry in high school. The visual module and rich theoretical material in the resource enable students of natural science specialties to more effectively learn the fundamental concepts of molecular symmetry, search for symmetry elements, and identify point groups of molecules. The results of a three-year implementation show a positive impact on student engagement in the course as well as academic performance. By using the Symotter resource, the students' level of mastery of the teaching material is consistently high at over 80%. A crucial role in the effectiveness of the study is played by the 3D visualization of molecular structures, symmetry elements and symmetry operations with the possibility of carrying out exercises for determining a point group of molecules both under the guidance of a teacher and independently. The resource provides invaluable assistance to both students and teachers in learning the concept of molecular symmetry.

Keywords: molecular symmetry, point groups, digital technologies, online-platform, methods of teaching chemistry, symmetry of molecules

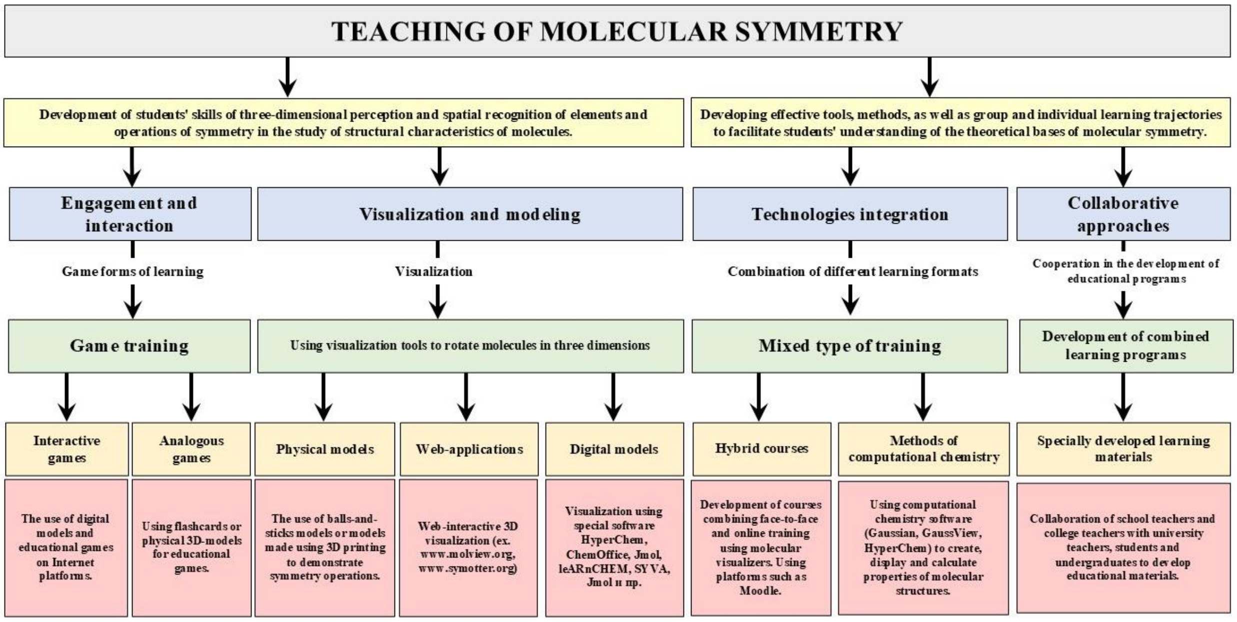
Introduction

The practical relevance of molecular symmetry to quantum chemistry (Pauncz, 2018) and molecular spectroscopy (Bunker & Jensen, 2006) makes it one of the major fields of chemical science. The study of molecular symmetry enables a deeper understanding of molecular properties and intermolecular interactions. The fundamentals of molecular symmetry include the study of symmetry elements and corresponding symmetry operations, which help students better understand the structural and optical properties of molecules. Although the concepts associated with molecular symmetry are not so difficult, their accurate understanding requires the use of a fairly serious mathematical apparatus and the provisions of group theory (Vázquez-Vidal, 1996). However, when molecular symmetry is taught in high school, there are several problems that make it difficult to understand what is, at first glance, quite difficult material, as there is currently no common system and uniform teaching methods of the molecular symmetry fundamentals.

The main difficulty in studying molecular symmetry is the need to visualize molecules in 3D from 2D images in order to find symmetry elements and operations that determine the belonging of a molecule in a particular point group (Rattanapirun & Laosinchai, 2023). Students often find it difficult to visualize the 3D shape of a molecule, especially in the early stages of familiarity with the concepts of molecular symmetry (Rattanapirun & Laosinchai, 2021). Furthermore, in many cases it is difficult to identify second-order axes (C_2), which perpendicular to axes C_n, and to find the σ_d planes that passing through the C_n axis dividing the angles formed by the neighboring C_2 axes in dihedral point groups (Chen и др., 2015). Therefore, the effective teaching of molecular symmetry requires a structured pedagogical approach that fosters both conceptual understanding and practical application. Fig. 1 presents a framework that reflects a multifaceted strategy aimed at developing students' three-dimensional perception and spatial recognition of symmetry elements in molecular structures.

Figure 1

Comprehensive pedagogical framework for teaching molecular symmetry.



To effectively learn the fundamentals of molecular symmetry, two main tasks must be solved:

- to develop students' skills in the 3D perception of molecular structures and
- to develop effective tools and methods to facilitate students' perception of the theoretical fundamentals of molecular symmetry.

To achieve these goals, the framework is organized into four key pedagogical components: engagement and interaction, visualization and modeling, technology integration, and collaborative learning approaches. Each of these components plays a critical role in reinforcing students' understanding of molecular symmetry by leveraging different teaching methodologies and tools.

In the context of molecular symmetry, game-based learning is employed to create an interactive and immersive educational experience. This approach encompasses both digital and physical learning tools. The integration of digital educational platforms, including interactive molecular modeling software and online games, allows students to explore molecular symmetry through engaging and visually stimulating activities. Such platforms enable real-time manipulation of molecular structures, reinforcing students' ability to recognize symmetry operations. Traditional educational games, such as flashcards and three-dimensional physical models, are utilized to supplement digital approaches.

Modern educational methodologies emphasize the integration of multiple learning formats. Blended learning approaches that integrate face-to-face instruction with online molecular visualization tools provide students with a flexible and comprehensive learning experience. Platforms such as Moodle facilitate the delivery of interactive course content. The development of effective educational programs benefits significantly from collaborative efforts between educators, researchers, and students. This framework promotes the co-development of learning materials and programs through interdisciplinary cooperation. This approach fosters a dynamic and inclusive learning environment that integrates theoretical knowledge with practical applications.

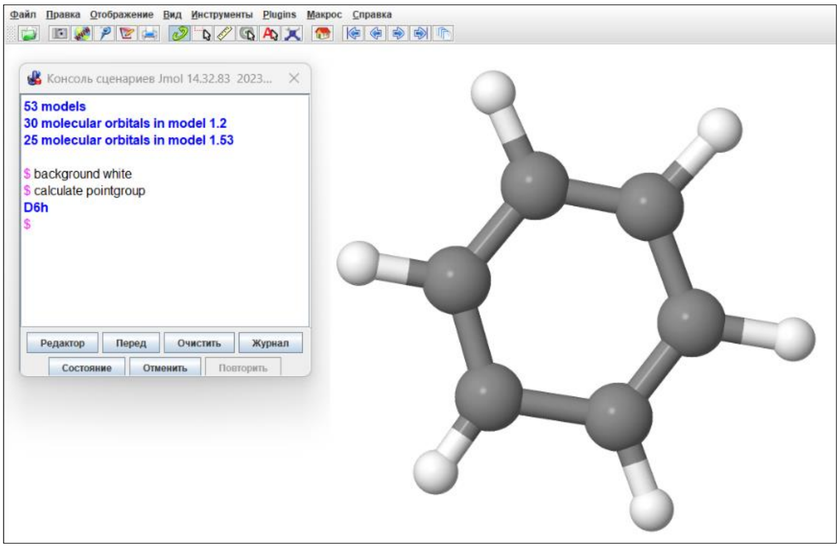
Given the inherently spatial nature of molecular symmetry, 3D visualization techniques are essential for facilitating students' understanding of symmetry operations. Ball-and-stick molecular models and 3D-printed structures serve as effective tools for demonstrating symmetry elements and their transformations. Such models provide students with a hands-on learning experience that enhances spatial reasoning skills. Online resources and advanced molecular visualization software provide interactive, web-based simulations that enable students to manipulate molecular structures and observe symmetry elements.

For these purposes, even before the emergence of mobile applications, various software products were developed (Meyer & Sargent, 2007), for example based on the ADDIE protocol (Korkmaz & Harwood, 2004) and even proposed to use the paper models (Sein, 2010). Some authors suggested the use of hybrid courses that combine online learning with traditional full-time courses (Antonoglou и др., 2011) or games (Dagnoni Huelsmann и др., 2018) or the use of models created with 3D printing (Savchenkov, 2020). The mobile augmented reality app leARnCHEM for symmetry visualization, developed in 2023, allows to search and animate molecules with symmetry elements and test the insights gained using quiz (Zambri & De Backere, 2024). The SYVA program has also been used to analyze molecular symmetry, which is compared with SYMMOL and molecule simulation programs such as NWChem or ORCA. SYVA can generate input files for molecular modeling programs and integrate them into GAMESS and MRCC (Gyevi-Nagy & Tasi, б. д.).

The program Jmol is also interesting - an interactive program for viewing molecular models on the computer (*Jmol: an open-source Java viewer for chemical structures in 3D. http://www.jmol.org/*). This open source program has long been used as a tool to study molecular symmetry (Cass и др., 2005). It is free for all users and can be successfully used to study molecular structures and develop training materials (Herráez & Herráez, 2007). However, Jmol is not a program for drawing structures. This requires another program, such as Spartan or Chem3D. To determine the point group of a molecule in Jmol, the appropriate "calculate pointgroup" command in the script console is required. After pressing the enter key, the result will be appeared in the next line, for example the definition of the point group for the benzene molecule (D_{6h}) (Fig. 2.).

Figure 2

Determination of the point group of a benzene molecule in the Jmol program.



The online resource Symmetry Resources at Otterbein University https://symotter.org has been successfully used for several years in the course “Contemporary perspectives on the structure of matter” in the master's program for studiyng the section “Molecular Symmetry". The resource is intended to make it easier for students and teachers to learn molecular symmetry and requires Microsoft Edge (Windows, macOS), Safari (macOS, iOS), Chrome (macOS, Windows, iOS, Android), or Mozilla Firefox (macOS, Windows, Linux, iOS, Android). The resource can be easily used on all types of digital devices: PCs, laptops, tablets, smartphones and interactive boards, without the need to install special software. At the same time, the device must have Internet access and a screen resolution of at least FullHD. To ensure complete and high-quality visualization, Symotter is accessible to students and teachers from anywhere and at any time, providing flexibility in learning, the ability to conduct online lessons and the opportunity to study learning material independently.

Even though traditional methods like using physical models or static diagrams are still useful, they have their limits because they can't represent the dynamic aspects of molecular symmetry. As an interactive online resource, Symotter offers significant advantages over traditional methods. It allows students to visualize and manipulate molecular structures in real time, improving material understanding and memorization. Unlike traditional methods where learning is often based on static images and models, Symotter provides dynamic and interactive learning that is more effective for understanding symmetry concepts. Symotter, on the other hand, allows students to experiment with various elements and operations of symmetry and immediately see the results of their actions, which contributes to the most comprehensive understanding and assimilation of the learning material.

This English-language resource, has intuitive navigation and contains several sections.

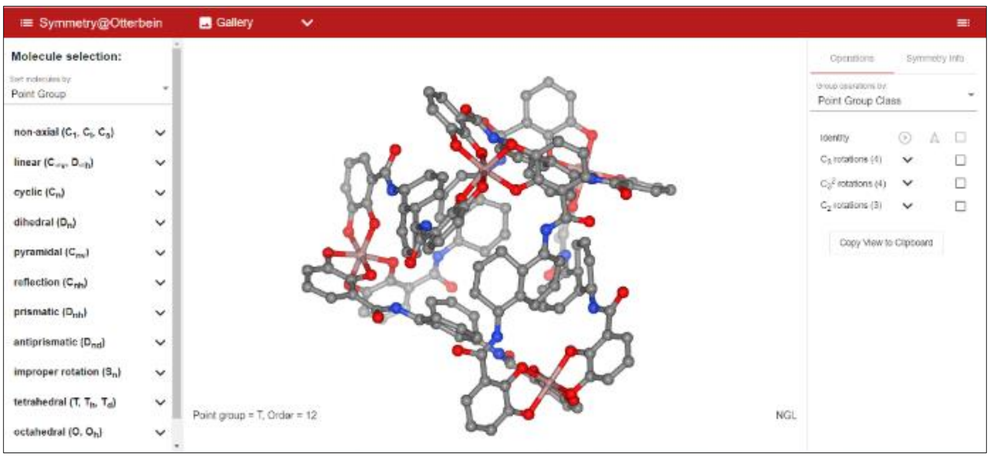
The “Tutorial” section briefly introduces the user to the elements and operations of symmetry. For a more detailed introduction to the theoretical foundations of molecular symmetry, the relevant literature is recommended (Bunker & Jensen, 2005; Hargittai & Hargittai, 2009; Pecharsky & Zavalij, 2005; Willock, 2009).

The "Gallery" section (Fig. 3A) contains an extensive collection of examples of different molecules for all 32 point groups. The data can be sorted by point groups, number of atoms, type of molecule, or in alphabetical order. The main feature of this section is the possibility of 3D visualization of elements and operations of symmetry, which, unlike paper or static models, allows a clear representation of the action of symmetry elements, which is useful for understanding the reversal and effect of mirror rotation axes. This gallery can also be used as an excellent lecture guide.

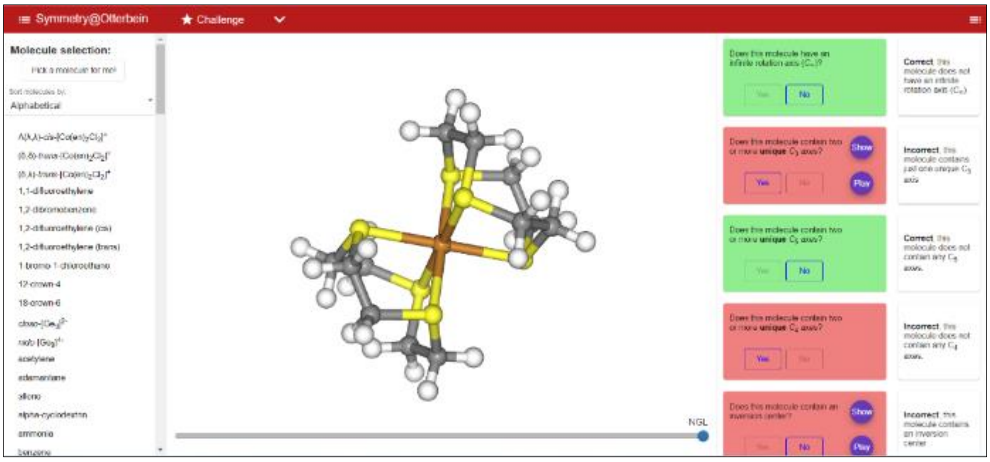
Figure 3

"Gallery" (A) and "Challenge" (B) sections of the online resource https://symotter.org

A



B



In the "Challenge" section (Fig. 3B), teachers can test students' acquired knowledge of defining the point group of a molecule. After clicking the "Pick a molecule for me" button, the system will automatically suggest one of the molecules present in the database and few consecutive questions to determine the point group. After all the answers have been completed, the system will prompt to verify their accuracy. Then, after clicking the "Check Answer" button, the system will highlight correct answers in green and incorrect answers in red. For each answer, a short explanation of the errors will also be receive. The "Show" and "Play" buttons visualize the corresponding elements and operations of symmetry. The functions of this section enable use in exams or interim controls.

Since the resource is English, it provides the opportunity to study the indispensable terminology in English, which must be done in the correct context when learning the discipline in Kazakh or Russian (Akatyev и др., 2023). Table 1 shows the basic terms in three languages for the section on molecular symmetry.

Table 1.

The fundamental terminology of the "Molecular Symmetry" section in three languages.

№	English	Kazakh	Russian
		Common terms	
1	Symmetry	Симметрия	Симметрия
2	Molecular symmetry	Молекулалық симметрия	Молекулярная симметрия
3	Point group	Нүктелік топ	Точечная группа
4	Symmetry group	Симметрия тобы	Группа симметрии
5	Group theory	Топтық теория	Теория групп
6	Symmetrical figure	Симметриялық фигура	Симметричная фигура
7	Representations of point groups	Нүктелік топ көріністері	Представления точечных групп
8	Representations of symmetry operations	Симметрия амалдарының бейнелері	Представления операций симметрии
		Symmetry elements	
9	Symmetry element	Симметрия элементі	Элемент симметрии
10	Symmetry axis	Симметрия осі	Ось симметрии
11	Inversion center	Инверсия орталығы	Центр инверсии
12	Rotation axis	Айналмалы ось	Поворотная ось
13	Mirror plane	Айна жазықтығы	Зеркальная плоскость
14	Plane of symmetry	Симметрия жазықтығы	Плоскость симметрии
15	Axis order	Ось реті	Порядок оси

16	Center of symmetry	Симметрия орталығы	Центр симметрии
17	Rotation-reflection axis	Айна-бұрылыс (инверсия) осі	Зеркально-поворотная (инверсионная) ось
Symmetry operations			
18	Symmetry operation	Симметрия амалы	Операция симметрии
19	Identity	Сәйкестік (ұқсас түрлендіру)	Идентичность (тождественное преобразование)
20	Rotation	Айналу	Вращение
21	Reflection	Шағылыс	Отражение
22	Inversion	Инверсия	Инверсия
23	Proper rotation	Меншікті айналым	Собственное вращение
24	Improper rotation	Меншікті емес айналу	Несобственное вращение

Methods and organization of the study.

As part of a control of the "Molecular Symmetry" section, master's students were asked to determine the point group of five molecules using the "Challenge" section of the Symotter source. Clicking the "Pick a molecule for me" button automatically select the molecule. To determine whether a molecule belongs to a particular point group, five questions had to be answered about the existence or absence of a particular symmetry element. It should be noted that when explaining the theoretical material in the lectures, the options in the "Gallery" section were used. The number of master's students in the academic years was: 15 in the 2021-2022 academic year, 16 in the 2022-2023 academic year and 12 in the 2023-2024 academic year.

The evaluation of the results was based on two criteria:

1) the number of specific point groups,

2) the total number of correct answers to questions for determining the elements of symmetry.

The need for such a distinction arises from the fact that to determine the point group of each molecule, all questions must be answered correctly. Even if one answer is wrong, it is not possible to determine the correct point group. However, at the same time, the student can correctly define several elements of symmetry. That is, if one mistake is made in three tasks, the student will not identify a point group for three molecules, but if three mistakes are made in one task—only one—and in both cases the same number of questions were answered. In this case, a student who identified more point groups will receive a higher score.

It should be clarified that the number of questions for determining a point group can range from 2 to 7, depending on whether the point group belongs to one or another category of symmetry. However, the number of questions is usually only five for most molecules in the resource database, which have between 4 and 20 atoms.

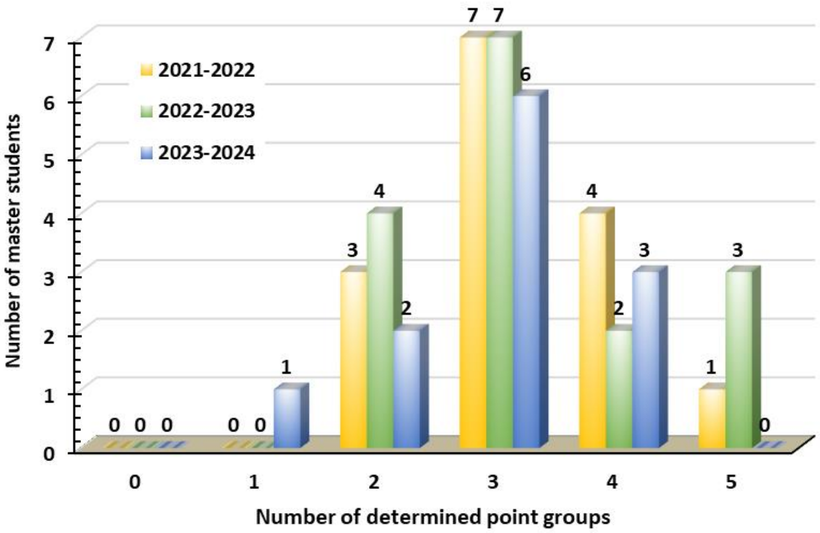
Results and discussion.

The analysis of the results of assessing the quality of knowledge of master's students according to specified criteria is shown in Figure 4.

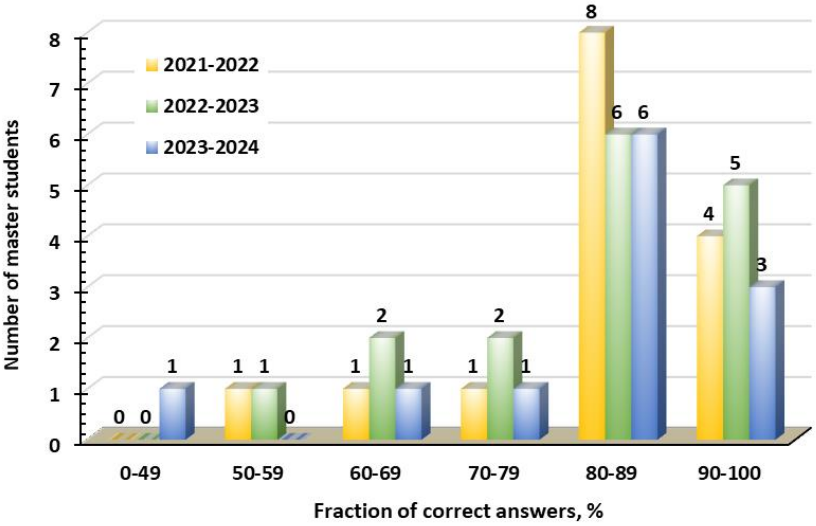
Figure 4

Results of assessing students' knowledge of the "Molecular Symmetry" using the Symotter online resource for three academic years: A - on criterion 1, B - on criterion 2.

A



B

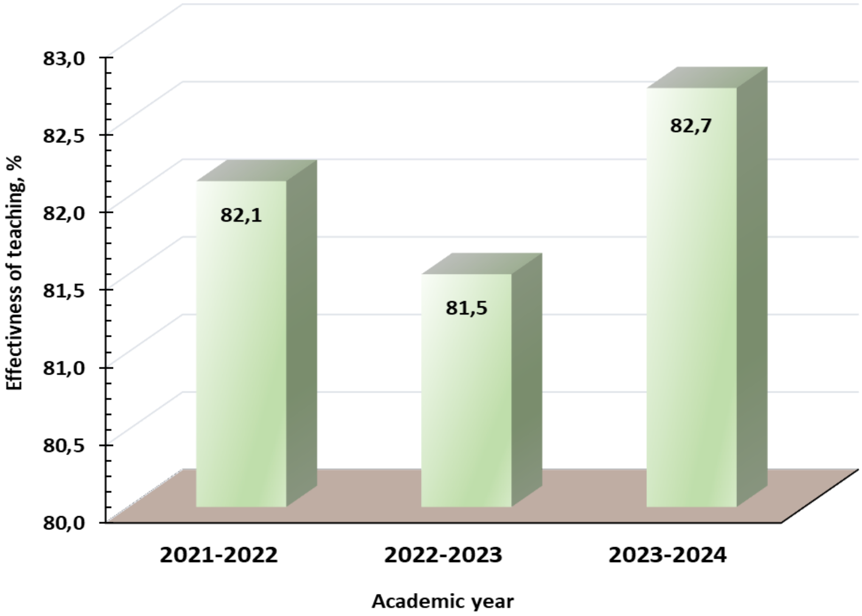


As can be seen, students are able to identify point groups of molecules and answer most of the questions asked, which is a very good indicator of the quality of learning. On average, each student is able to identify point groups of three out of five molecules. For molecules belonging to the lower and middle symmetry categories as well as special point groups ($C_{\infty v}$, $D_{\infty h}$), symmetry elements and point groups are easy for students to identify, while highly symmetric molecules belonging to a higher symmetry category sometimes cause difficulties.

The effectiveness of learning the fundamentals of molecular symmetry using the online resource Symotter over three academic years is shown in Figure 5.

Figure 5

The effectiveness of teaching the fundamentals of molecular symmetry using the Symotter online resource.



The results clearly demonstrate that using the Symotter online resource while learning the fundamentals of molecular symmetry leads to a very stable understanding of the subject by more than 80%. Additionally, a survey of students indicates that everyone finds this resource very useful and effective. The main advantages are intuitive navigation and excellent visualisation of symmetry elements and operations, as well as the possibility of making full use of the resource from any digital device, anywhere.

Conclusion

The use of digital tools promotes a deeper understanding of molecular symmetry aspects and provides students with the basic spatial reasoning and analytical skills that are essential for their future studies in chemistry and related fields. The Symotter online resource is a simple, affordable, and powerful tool for learning the fundamentals of molecular symmetry that can complement and exceed traditional methods due to its interactivity and ability to provide insightful and practical learning. Symotter is a learning platform that helps students learn about the elements and operations of symmetry and determine the point group of molecules, which is essential for understanding the properties of molecular structures. This approach improves the quality of knowledge and stimulates students' interest and involvement in the study of the subject, which further leads to better learning outcomes in other chemistry fields that use the concepts of molecular symmetry. To improve Symotter's educational capabilities, the developers plan to further integrate augmented reality technologies, which can significantly improve learning methods and provide full-fledged 3D interactive immersion in the learning environment.

Conflict of Interest Statement

The author declare no potential conflicts of interest regarding the research, authorship, or publication of this article.

The use of artificial intelligence (AI)

During the preparation of the manuscript, the capabilities of AI were used to search and analyze references and perform preliminary language editing.

Author contributions

The author confirms the sole responsibility for the conception of the study, presented results and manuscript preparation.

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