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Transforming Chemistry Education through Digital Tools: Enhancing 3D Visualization and Conceptual Understanding

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Abstract

Chemistry is inherently a three-dimensional (3D) science, yet it is often taught using traditional two-dimensional (2D) methods such as black boards, whiteboards, and textbooks. This mismatch creates a “conceptual gap” for students, particularly in areas like molecular symmetry, solid-state chemistry, and stereochemistry. This paper explores the use of interactive 3D visualization tools such as Jmol, ChemTube3D and Symmetry@Otterbein in the classroom to enhance molecular understanding. These tools allow students to rotate, reflect, zoom, and perform symmetry operations and identify point groups in real time. Using Jmol open-source 3D molecular viewer, students can visualize and analyze molecular symmetry and point groups with the help of console commands. By utilizing the “Show All Symmetry Elements" in the control tab of Chemtube3D, students can find out individual symmetry operations and identify the point group. The resources included in Symmetry@Otterbein web-based educational tool are specifically designed to help students learn molecular symmetry concepts and to aid teachers in providing live demonstrations of topics that are challenging to convey through verbal explanations, hand-drawn illustrations, or even physical models. By incorporating these tools into the classroom, students can develop a more intuitive and practical understanding of complex concepts. At the same time, teachers can transform their pedagogy from passive lecturing to a dynamic, interactive, and student-centered approach, thereby fostering deeper understanding and improved retention of challenging chemical concepts.

Keywords: Active Learning, Chemistry Education, Digital Tools, Molecular Symmetry, 3D Visualization

Introduction

Chemistry forms the foundation for understanding many other scientific fields, including biology, physics, geology, materials science, and environmental science. In order to enhance students' comprehension of chemistry concepts and theories in a variety of contexts such as molecular symmetry, solid-state chemistry, and stereochemistry, 3D visualization digital tools should be included into chemistry education. The use of these powerful tools in teaching chemistry education to enhance student learning process and it is necessary to discuss about the incorporation of these tools into teaching and learning processes for offering innovative ways of teaching (Kubiliene et al., 2024). The inclusion of digital tools in the educational sphere brings new cognitive activities into practice, as they are highly interactive and practical in the classroom. Digital tools enable the construction of knowledge, facilitate interaction and stimulate students towards meaningful learning. In the 21st-century digital era, Teachers are in a position to expand their digital knowledge and use digital tools in teaching to create a student-centered transformative approach and enhance student's learning processes (Nino, 2023).

Review of Related Literature

The present study explores the use of new digital technologies in the teaching of Group Theory in Chemistry, focusing on active methodologies that seek to overcome the traditional teaching model. The main objective was to understand how digital technologies can improve the teaching-learning process of Symmetry concepts in Group theory. 3D visualization tools are a game-changer for teaching molecular symmetry, a topic that faces challenges using 2D paper diagrams. The challenges include identifying symmetry elements (□-plane of symmetry, Cn-proper axis of rotation, Sn-improper axis of rotation and i-centre of symmetry) and determining point groups. By moving beyond static images, these tools transform how students understand the mathematical and physical balance of molecules. This paper explores the use of interactive 3D visualization tools such as ChemTube3D, Jmol, and Symmetry@Otterbein(symotter.org) in the classroom to enhance molecular symmetry understanding. These tools allow students to perform all symmetry operations such as rotation, reflection, inversion in real time and identify point group and list down all symmetry elements present in any molecule.

Objectives

This paper explains the different 3D visulalization tools used for teaching symmetry concepts with animation. ChemTube3D, Jmol, and Symmetry@Otterbein(symotter.org) tools are particularly used for teaching molecular symmetry in 3D view with animation and make students to develop a more intuitive and practical understanding of symmetry concepts in group theory.

Methodology

ChemTube3D is an Open Educational Resource (OER) that contains interactive 3D chemistry animations and structures. ChemTube3D.com has been available to the educators and learners as an Open Educational Resource since January 2008. The number of symmetry elements such as axis of rotation (Cn), plane of symmetry (□v , □h and □d), centre of Symmetry(i), and improper axis of rotation(Sn) present in any molecule can be found out, by clicking Symmetry under Structure and Bonding menu on ChemTube3D. (Figure 1).

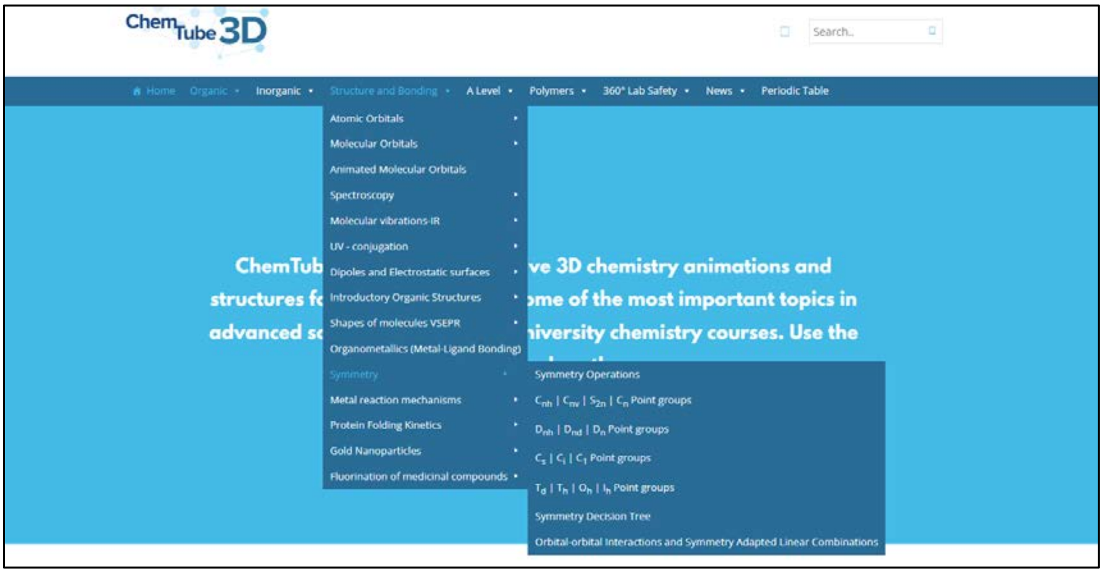

Figure 1: Selection of Molecule on ChemTube3D

Analysis

After selecting the molecule (for an example, Octahedral SF_6 molecule under Oh), we can get the following window showing the structure of SF_6 with options to be chosen for viewing symmetry elements and animation (Figure 2).

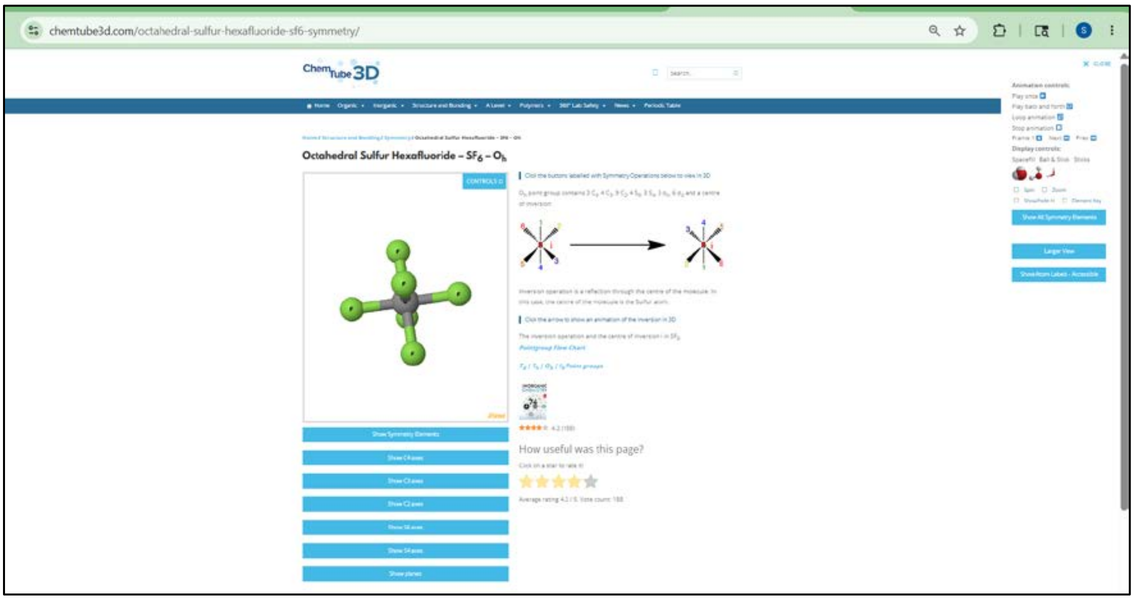

Figure 2: Visualization of symmetry operations in ChemTube3D

Using the "Controls" button, detailed examination of the animation of the molecule for each symmetry operation can be viewed and the "Show Larger View" button gives larger view as well as controls for the animation and display. Total number of symmetry elements can be found out by using all symmetry element button. The molecule can be rotated using mouse and shifting of atoms for each rotation can be easily visualized.

Similarly, Jmol can also be used to view the 3D animation of molecules for each symmetry elements present in it. Jmol is an Open Source molecular viewer licensed under the GNU Lesser General Public License. Jmol is a Java applet that is emerging as a suitable replacement for both RasMol and Chime (which were used as tools for viewing the three dimensional structures of molecules in the mid to late 1990's. Jmol is a free and open source computer visualization powerful program and runs on a Java platform. It is being used as a teaching tool by teachers, researchers and scientists to visualize a molecule in 3D space. Jmol is used either as an independent program by downloading like any other program on a desktop and functions equally well in a PC or Mac environment or as a web application. Jmol has a web-based version (i.e."JSmol") that runs on a JavaScript platform and functions equally well on all HTML5 compatible browsers such as Firefox, Internet Explorer, Safari and Chrome. In Jmol window, at first, the structure of the molecule is obtained by typing the molecule name (for example, Methane - CH4) in input window from "Get Mol" under File menu and the atoms are numbered by choosing label option and the structure is shown in Figure 3.

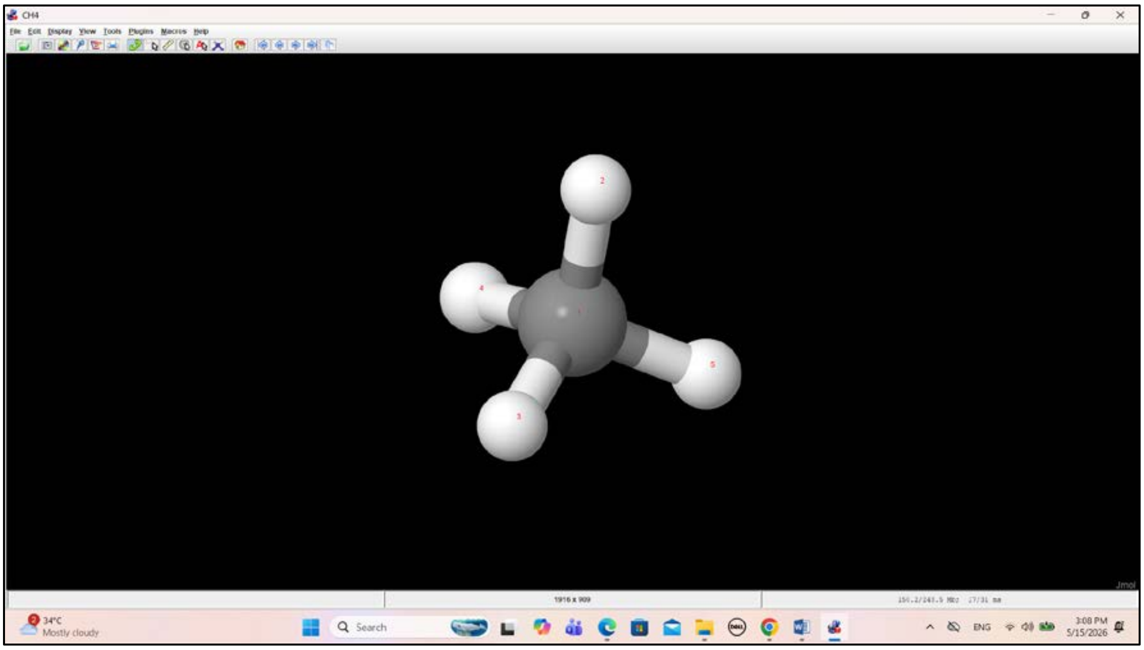

Figure 3: Visualization of CH_4 in Jmol

By giving proper commands (always start with $) in console window, molecules can be rotated about an axis or reflected by choosing a plane and inverted about a point(centre) and point group of any molecule can be easily determined. For example by the giving the following command "$ draw plan 1 300 plane (atomno=1) (atomno=2) (atomno=3)" for methane (CH_4) molecule in Jmol, we get the following image showing the plane having atoms 1(carbon) and atoms 2 and 3(hydrogen atoms) and the image is shown in Figure 4. In a similar way, by giving proper commands in console window, user can add more number of planes with different colours for easy understanding. Animations for reflection and rotation can also be done in real time using Jmol by giving proper commands in Console window.

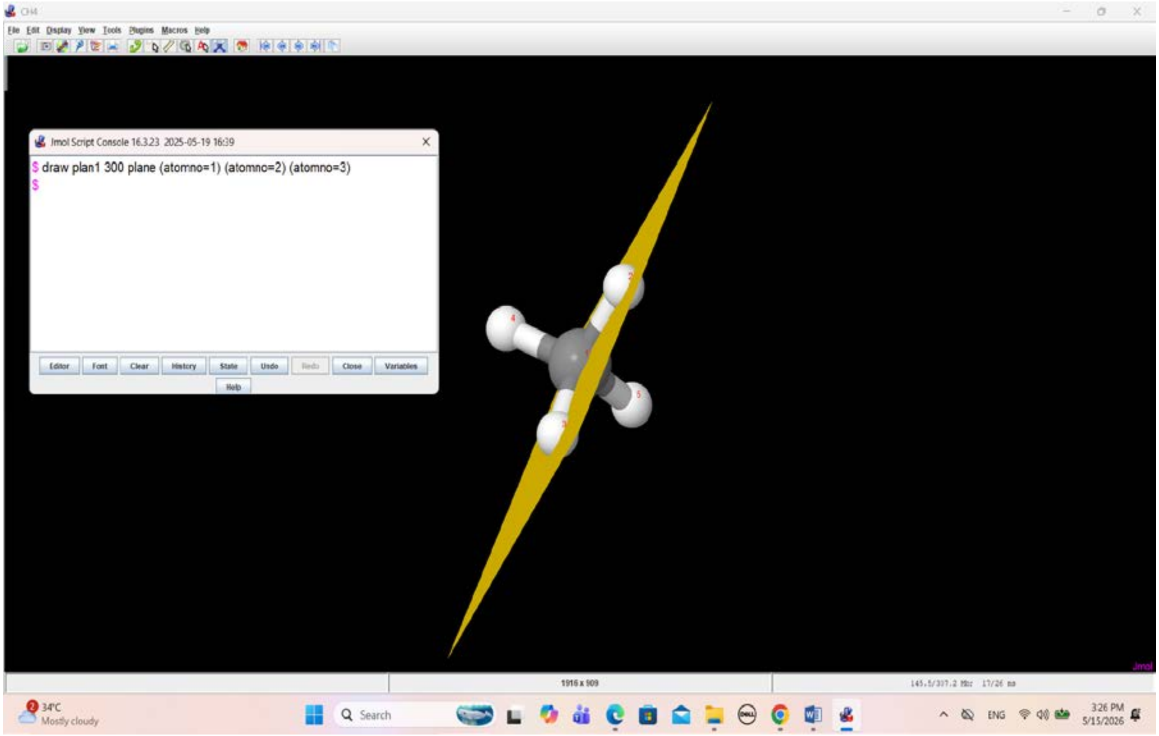

Figure 4: Visualization of Jmol Script Console window with command CH_4 in Jmol

Similarly Symmetry@Otterbein(symotter.org) can also be used as a digital tool to view molecules in 3 Dimension in real time. Symmetry@Otterbein(symotter.org) is a web-based educational tool which helps teachers in providing live demonstrations of different types of symmetry elements and operations and make students to learn about symmetry concepts in group theory. In the Symmetry Gallery of symotter.org has a collection of over 120 unique molecules and polyhedra with interactive display of all symmetry elements and animation of all operations. The molecules are organized by point group in such a way that the user can select examples to demonstrate particular symmetry elements.

Findings and Discussion

Using 3D digital tools teachers can teach the complex and confusing concepts of symmetry elements to students in an attractive way by having them explore to use these tools and learn by hands-on training. For example, to explain the presence of different symmetry elements in Molecules having similar formula but different geometry, ChemTube3D is very useful. For an example consider AB3 type molecules having different geometry. While teachers often find that using 2D methods to teach symmetry elements in AB3 type molecules, such as pyramidal NH3 (Ammonia) and trigonal planar BF3 (Boron trifluoride) to students with 2D methods, teachers found it very difficult to make the students to understand the concept. But when the same concept is taught by utilizing ChemTube3D (a 3D visualization and animation tool), it significantly enhances the interaction and allows students to grasp concepts like rotation axes and reflection planes with greater clarity. For example, consider the determination of symmetry elements present in a non-planar Ammonia molecule (NH3) using ChemTube3D tool. From the ChemTube3D window, one can easily find out how the atoms (N &H) in ammonia molecule shift their position when the molecule is rotated through C3 axis (Figure 5) through animation, reflected through reflection (mirror) plane (□v) (Figure 6) and all the symmetry elements present in ammonia molecule (Figure 7) excluding identity operation (E).

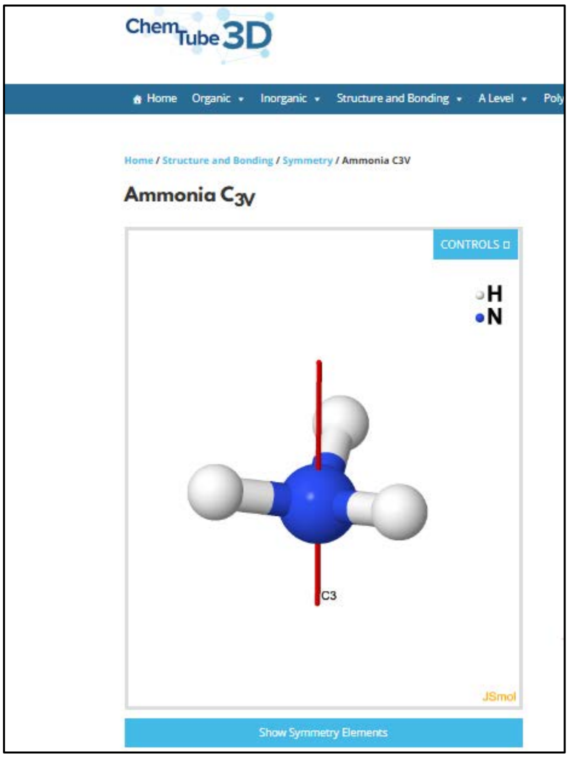

Figure 5: ChemTube3D image of C_3 axis of Rotation in NH_3

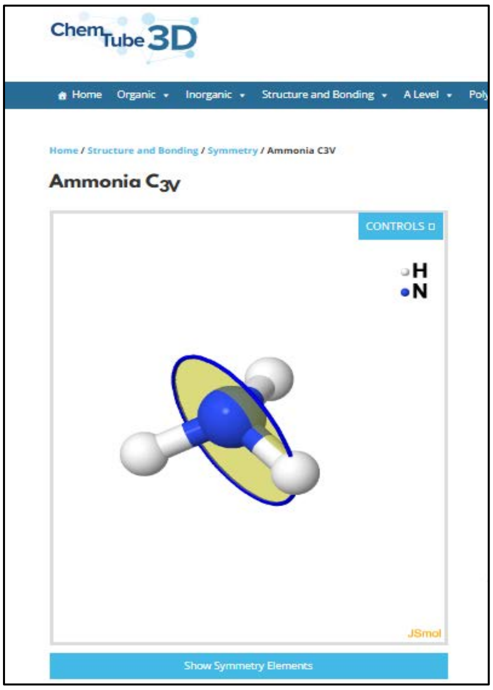

Figure 6: ChemTube3D image of Reflection (mirror) planes (σ_v) in NH_3

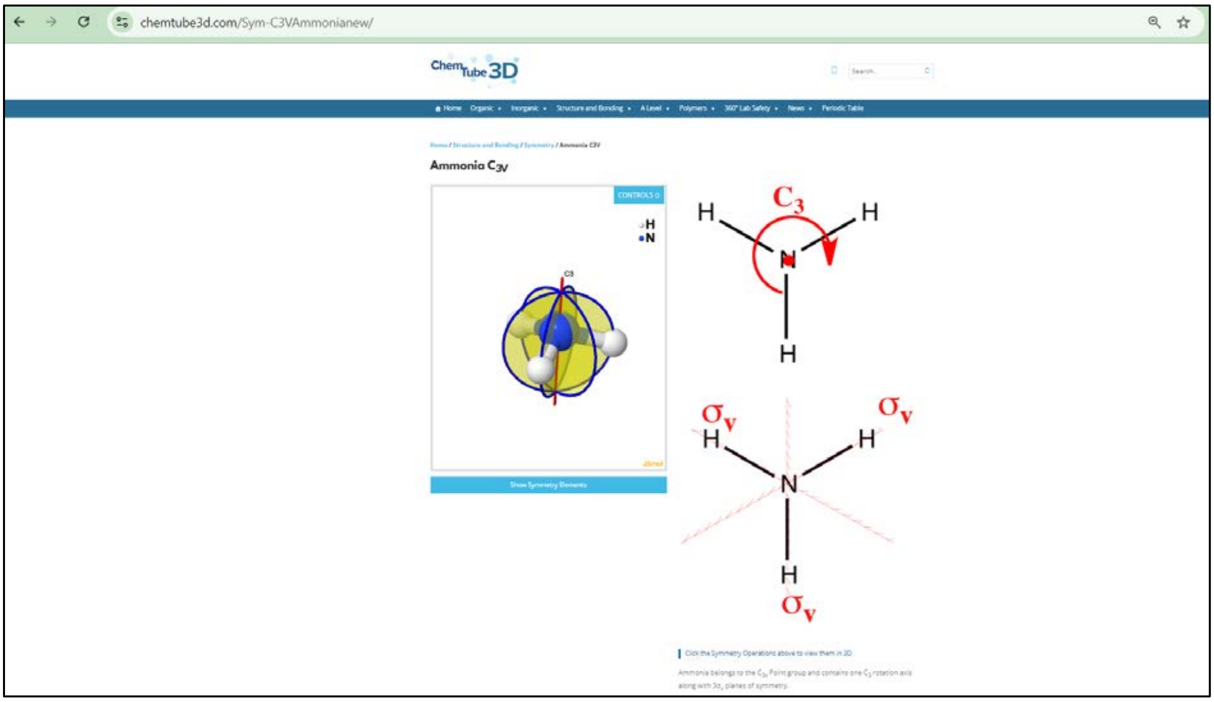

Figure 7: ChemTube3D image of Symmetry elements (C_3 & $3\sigma_v$) of NH_3

Similary, the symmetry elements present in planar Boron trifluoride (BF_3) molecule can be clearly explained by using ChemTube3D. Teachers can easily differentiate between C_3 axis of rotation (Figure 8) and three C_2 axes of rotation (Figure 9) and σ_h plane and three σ_v planes (Figure 10) and through animation in ChemTube3D window.

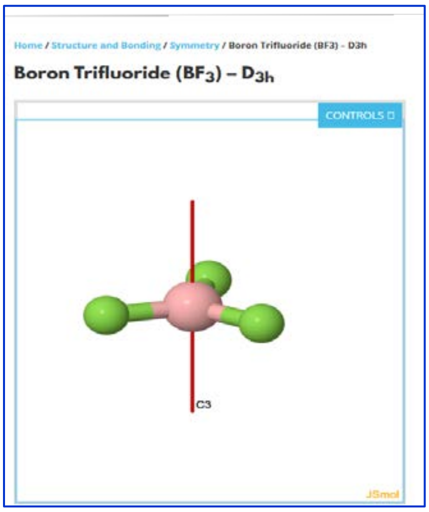

Figure 8: ChemTube3D image of C_3 axis of Rotation in BF_3

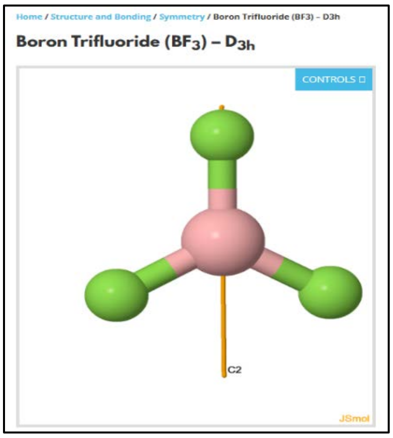

Figure 9: ChemTube3D image of C_2 axis of Rotation in BF_3

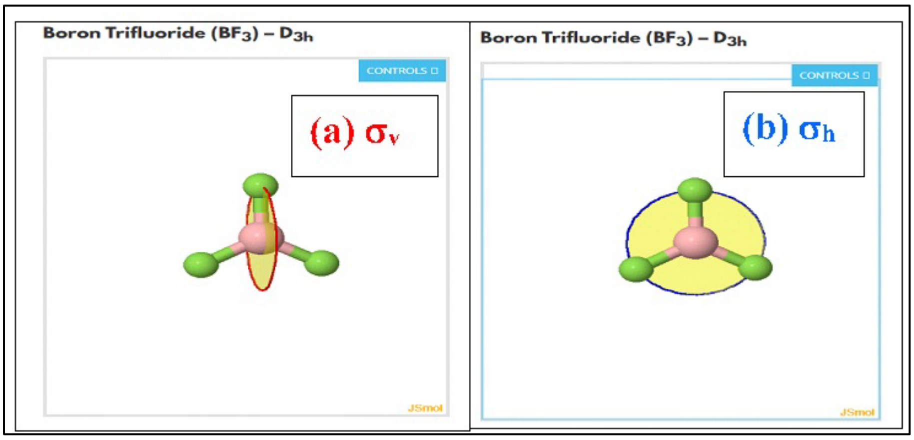

Figure 10: ChemTube3D image of Reflection (mirror) planes in BF_3 (a)σ_v, (b) σ_h

All symmetry elements present in BF_3 is shown in Figure 11 and from the image, user can easily list down the symmetry elements and determine the point group using ChemTube3D.

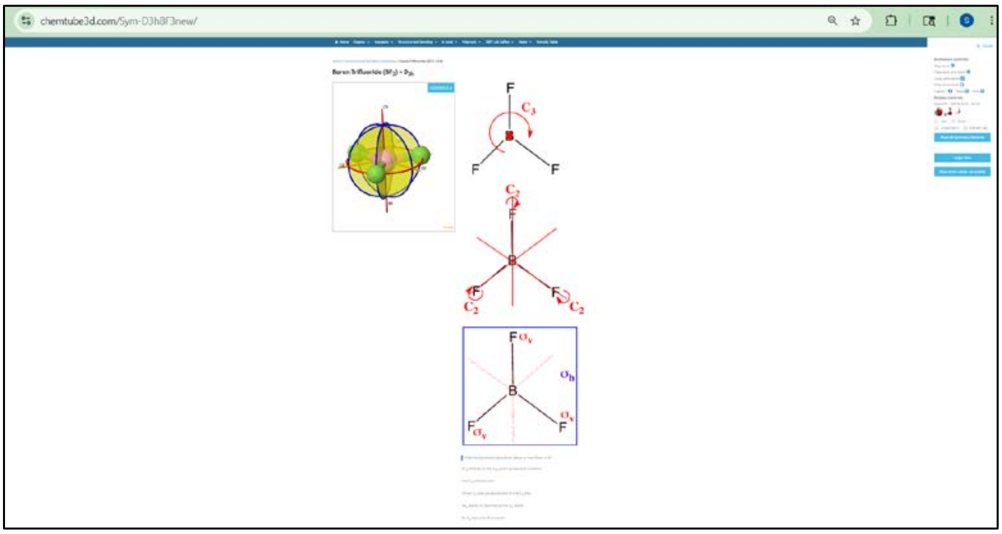

Figure 11: ChemTube3D image of Symmetry elements (C_3, $3C_2$, $3\sigma_v$ and σ_h) in BF_3

Thus by using ChemTube3D tools, teachers can make students to understand clearly unlike Boron trifluoride, Ammonia molecule does not have C2 axis of rotation and □h plane because of non-planar geometry but have C3 axis of rotation and 3□v planes only along with Identity(E) using animation and 3D view.

Similarly by using Jmol digital tool, symmetry elements of molecules can be viewed 3 dimensionally with animation by giving proper commands in Console under File menu. For example, the images obtained for one of the □v plane, C3 axis of rotation, and all symmetry elements present in CH4 by using Jmol open source are shown in Figure 11,12 and 13.

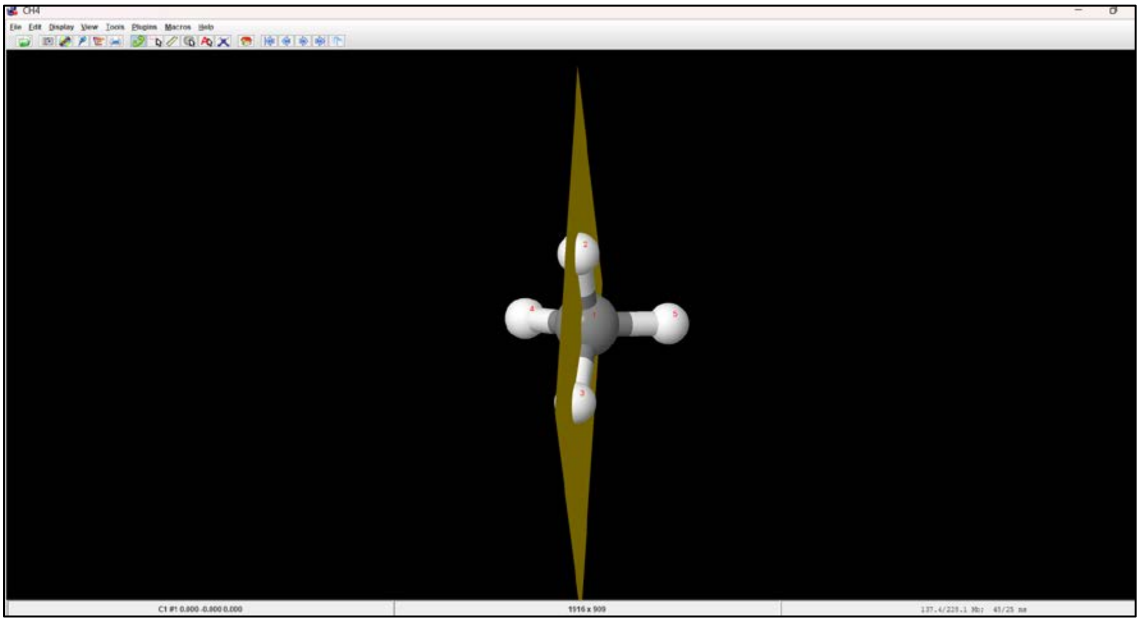

Figure 12: Visualization of a σ_v plane of CH_4 in Jmol

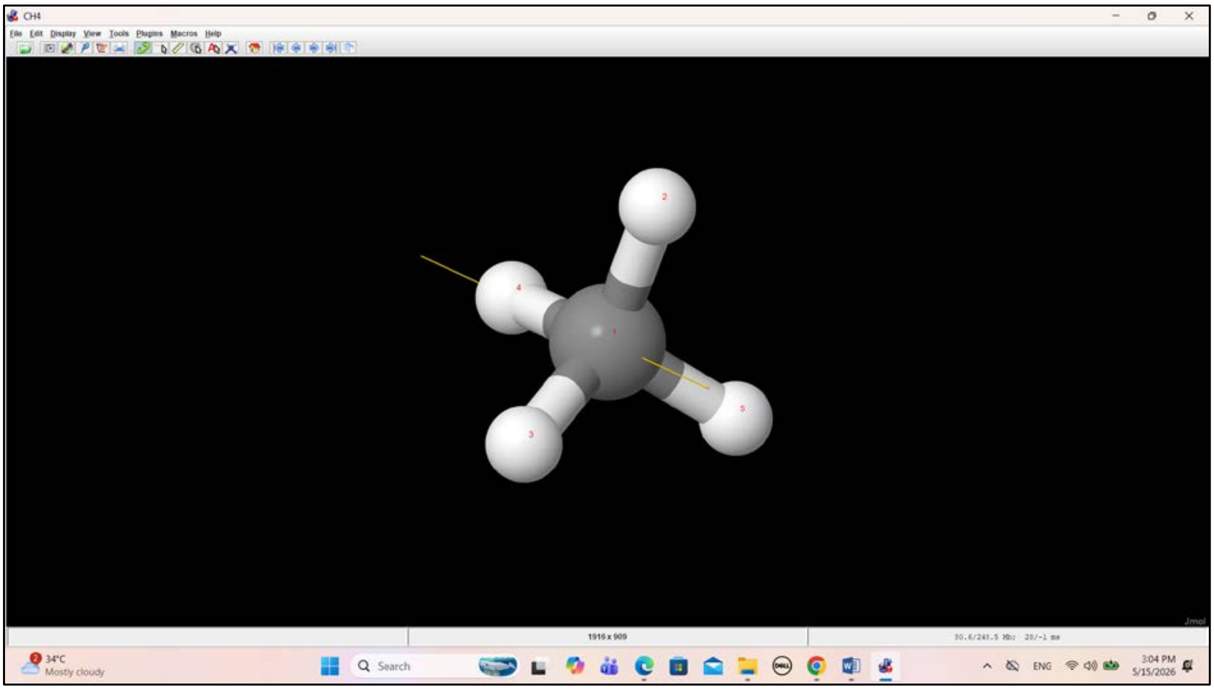

Figure 13: Visualization of C_3 axis of rotationof CH_4 in Jmol

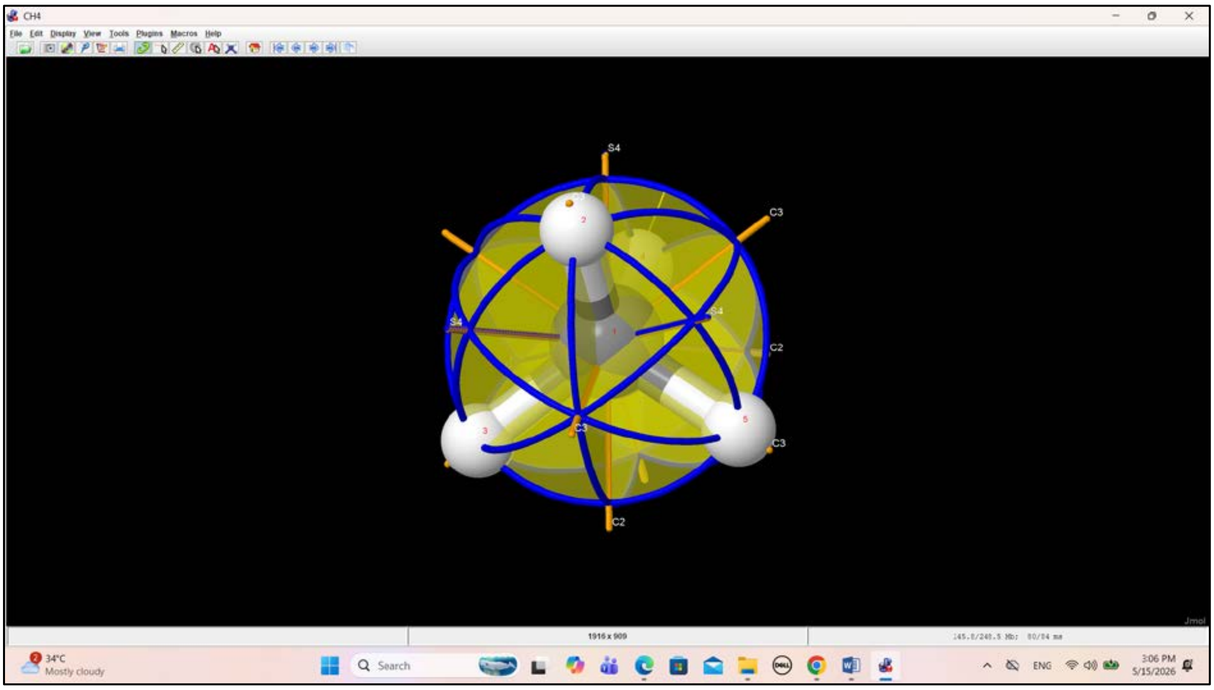

Figure 14: Visualization of allrotation and reflection symmetry elements of CH_4 in Jmol

Likewise, Symmetry@otterbein(symotter.org) can also be used to view molecules in 3D with animation for each symmetry elements present in a molecule and determine point group. Using the symmetry challenge option in symotter.org, for the same set of molecules in the Gallery, a flow chart showing the details of determining the point group of each molecule can be easily done by hands-on experience and it is found to a great and interesting way to practice the point group determination process. From the Symmetry gallery option in symotter.org, symmetry elements of the molecule to be determined are chosen and by clicking Operations and Symmetry Info tabs, user can view the structure with animation and number of symmetry elements present in it. For example, the structures obtained for the symmetry elements of chloromethane molecule(CH3Cl) from Operations and Symmetry Info tabs is given in Figures 12,13 and 14. Chloromethane molecule is chosen and the images of C3 rotational axis (Figure 12), □v (reflection/mirror) plane (Figure 13) and all the symmetry elements excluding Identity ((Figure 14) with point group of chloromethane and students can easily learn these symmetry elements with animation along with Vibrational representations.

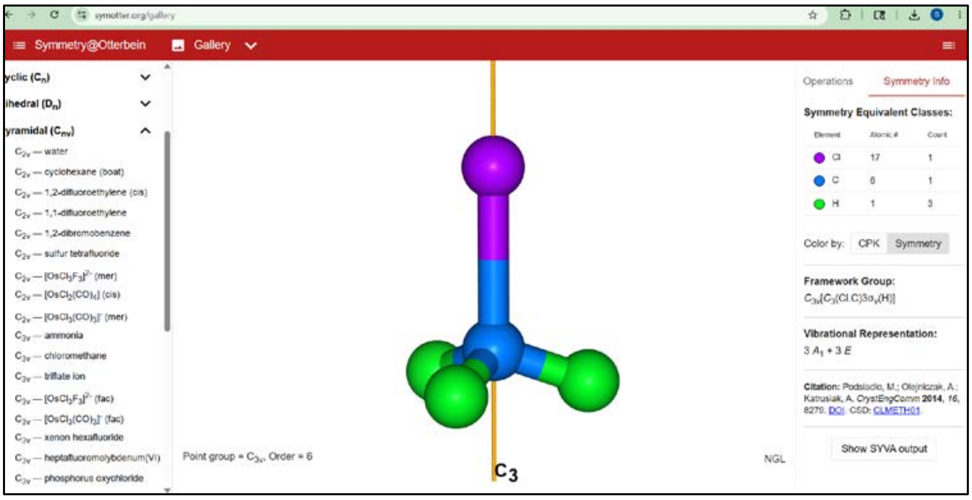

Figure 15: Structure of CH_3Cl showing C_3 axis of rotation visualized using Symmetry@Otterbein (symotter.org).

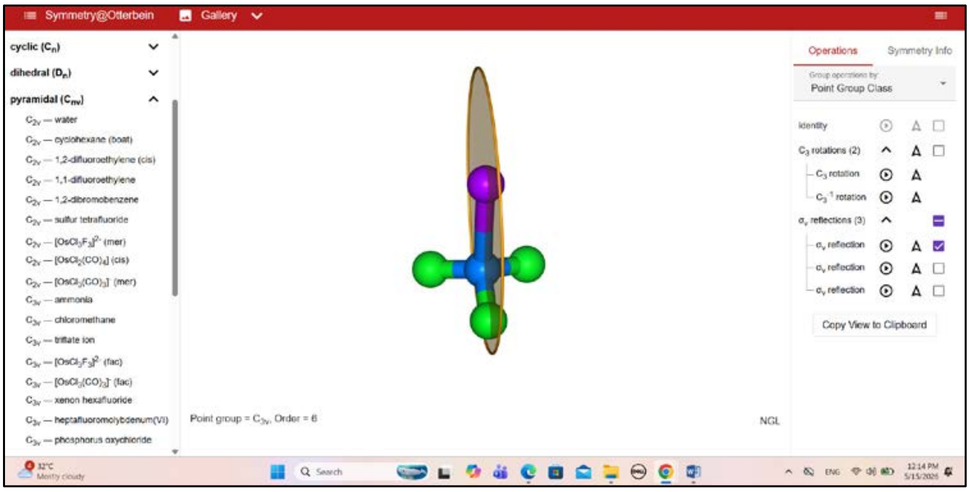

Figure 16: Structure of CH3Cl showing σ_v plane visualized using Symmetry@Otterbein (symotter.org).

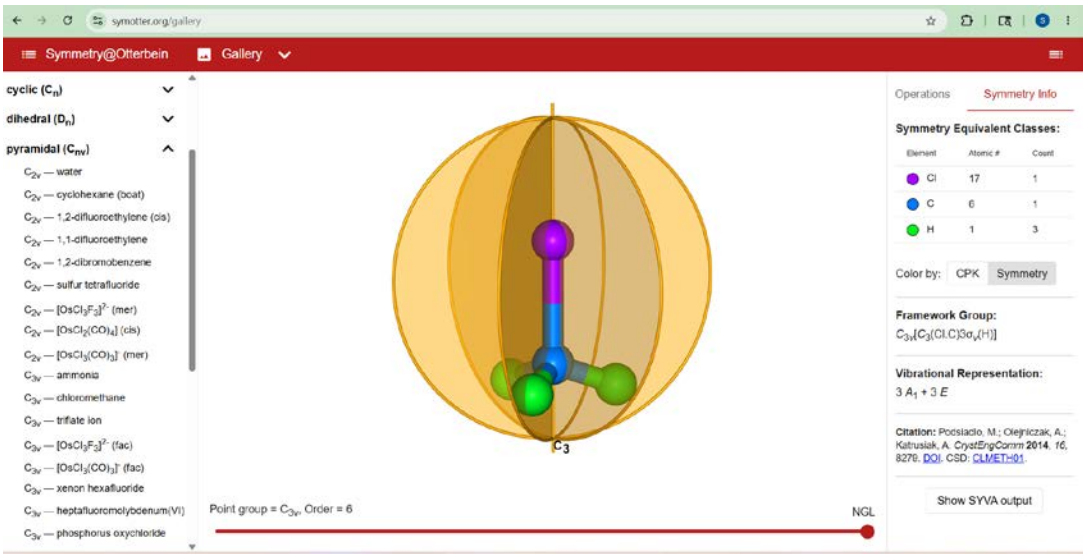

Figure 17: Structure of CH_3Cl showing C_3 axis of rotation and 3 σ_v planes visualized using Symmetry@Otterbein (symotter.org).

For explaining all symmetry elements in this paper, only images can be shown and 3D animation is not possible show since this paper is in 2. But while using the above three tools in class room, users can view the 3D image with animations in real time.Thus, by using these 3D visualization tools, teachers can transform their teaching pedagogy from passive lecturing to a dynamic, interactive, and student-centered approach, thereby fostering deeper understanding can make students to use these tools to determine the symmetry elements and point group of all molecules.

Conclusion

This paper demonstrates that the integration of ChemTube3D, Jmol and Symmetry@Otterbein(symotter.org) tools as 3D Visualization and animation Tools for teaching Symmetry concepts meaningfully in chemistry education by enhancing students' conceptual understanding. The use of these digital tools bridges the gap between symbolic representations and deeper conceptual understanding of symmetry elements by providing interactive 3D visualizations that allow users to actively manipulate molecular symmetry, overcoming the limitations of 2D diagrams. These findings highlight the importance of 3D visualization tools in Chemistry Education to promote active, dynamic, effective, constructive and interactive learning environment leading to improved learning outcomes and a more profound appreciation of Chemistry education.

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