Predicting the point group of molecules using Jmol application

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Abstract

The knowledge of symmetry and point group of molecules play a key role in understanding the physical and chemical characteristics of the molecules relevant to its applications. The details of point groups of any molecule provide a systematic technique to define the symmetry of molecules. This knowledge aids in predicting a variety of physical and chemical features, including molecule polarity, spectroscopic behaviour, and reaction process. For example, it helps to determine a molecule's vibrational modes and optical activity, which are important in fields such as materials science, drug design, and catalysis. A point group defines all of the symmetry operations that can be performed on a molecule to get a conformation that is indistinguishable from its original. A point group in chemistry and crystallography is a set of symmetry operations that leave at least one point fixed in space. These procedures include rotation and inversion. Point groups are used to categorize molecules and crystals according to their symmetry features. The 3D viewing of the molecule   offers a better platform for understanding the concept of symmetry and point group. The Jmol application, an open source software is user friendly and provides the learners a complete guide to predict the point group of the wide variety of molecules. The level of learning improved drastically using the 3D viewer like Jmol compared to the traditional methods. It enables better visualization of how molecules or crystals behave under various symmetry operations. In this report we have discussed how to predict the point group of various molecules using Jmol, by taking one molecule as an example for each point group.

Keywords

Point group, symmetry, rotation, axis, Jmol, 3D Visualization

Introduction

Understanding the symmetry of molecules is very important in chemistry because it helps explain many of their properties and behaviours. Classifying molecules into point groups, which describe their symmetry, is a key task in studying molecular structure and reactions. To predict the point group of molecules using Jmol, a free tool that allows scientists to see and analyse molecules in 3D. Jmol is widely used because it's powerful tools and easy to use features, making it perfect for this project. The main goal of my project was to create a reliable way to predict the point group of different molecules using Jmol. To do this, I needed to understand the basics of point group theory, learn how to use Jmol effectively, and develop scripts to make the process automatic. Understanding molecular symmetry and point groups is fundamental in chemistry as it provides a framework for predicting molecular behaviour and interactions. By using tools like Jmol, chemists can visualize and analyse molecular symmetry more efficiently, aiding in research and education.

The project was divided into several key steps:

1. Learning the Basics: Understanding the theory behind molecular symmetry and how point groups are classified. This involved studying the different point groups and their characteristics.

2. Getting to Know Jmol: Learning how to use Jmol, setting up the software, and exploring its features related to symmetry analysis.

3. Developing the Method: Creating a step-by-step method to identify and classify the point group of a molecule using Jmol. This included writing and testing scripts to automate the process.

4.Testing the Method: Applying the method to different molecules to see if it works correctly. Comparing the results with known point group classifications to make sure it's accurate.

5.Report Writing: Documenting the whole process and writing a guide to help others use Jmol for point group prediction in the future.

Completing this project helped me learn a lot about molecular symmetry and how to use computational tools in chemistry. This report will explain the methods I used, the challenges I faced, the results I got, and what I learned from this experience.

Basics of Molecular Symmetry and Point Groups

● *Introduction to Molecular Symmetry*

Molecular symmetry refers to the spatial arrangement of atoms in a molecule that results in a balanced and proportionate structure. Symmetry is an important concept in chemistry because it helps predict and explain the physical and chemical properties of molecules, such as their reactivity, polarity, and spectral characteristics.

● *Symmetry Elements and Operations*

A molecule is considered symmetrical if it can undergo certain symmetry operations and still appear unchanged. These symmetry operations are associated with specific symmetry elements. The main symmetry elements and operations are:

1. Identity (E): The simplest symmetry element, where the molecule remains unchanged. Every molecule has at least this symmetry.

2. Rotation Axis (C_n) axis around which the molecule can be rotated by (360°/n) and look the same. For example, a C_2 axis means a 180°rotation results in an identical appearance.

3. Mirror Plane (σ): A plane that divides the molecule into two mirror-image halves. If the molecule looks the same on either side of the plane, it has a mirror plane symmetry.

4. Inversion Center (i): A point at the center of the molecule where if all parts of the molecule are inverted through this point, the molecule looks the same.

5. Rotation-Reflection Axis (S_n): A combination of rotation about an axis and reflection through a plane perpendicular to that axis. For example, an S2 operation involves a 180°-degree rotation followed by reflection.

● *Point Groups*

Point groups are classifications of molecules based on their symmetry elements. Each point group has a set of symmetry operations that describe the symmetry of the molecule. Some common point groups are:

1. *C_n:* Molecules with a single n-fold rotation axis. For example, ammonia (NH_3) belongs to the C_3 point group because it can be rotated 120 degrees around its central axis.

2. *D_n:* Molecules with an n-fold rotation axis and n perpendicular C2 axes. For example, ethane (C_2H_6) in its staggered conformation belongs to the D3d point group.

3. *S_n:* Molecules with an n-fold rotation axis combined with a perpendicular mirror plane. For example, certain chiral molecules may belong to this group.

4. *C_s and C_i:* C_s includes molecules with a single mirror plane, while Ci includes those with an inversion center.

5. T_d, O_h, T_h: Highly symmetrical point groups. T_d includes molecules like methane (CH_4) with tetrahedral symmetry, O_h includes molecules like SF_6 with octahedral symmetry, and T_h includes molecules with icosahedral symmetry.

● *Determining the Point Group*

To determine the point group of a molecule, follow these steps:

Step 1. *Identify All Symmetry Elements:* Look for all the symmetry elements present in the molecule.

Step 2. *Use a Flow Chart or Table:* Follow a systematic approach or use a flow chart that guides you through questions about the symmetry elements to arrive at the correct point group.

Step 3. *Check Against Examples:* Compare the molecule to known examples of point groups to confirm your classification.

Identify All Symmetry Elements

Identifying symmetry elements in a molecule involves recognizing the various types of symmetry operations that leave the molecule unchanged. These symmetry elements help describe the overall symmetry of the molecule, which is crucial for understanding its properties and behavior. Here are some common symmetry elements and how they can be identified:

1. **Mirror Plane (σ)**:
   - A mirror plane is a flat surface that divides the molecule into two equal halves, reflecting one half onto the other.
   - To identify a mirror plane, visualize whether the molecule has a plane of symmetry where one half of the molecule mirrors the other.
   - Examples: Ethane (C_2H_6) has a mirror plane perpendicular to the C-C bond.

2. **Rotation Axis (C_n)**:
   - A rotation axis is an imaginary line around which the molecule can be rotated by a certain angle (360°/n) and remain unchanged.
   - Identify the axis by finding a line through the molecule around which rotation by a specific angle (n) produces an indistinguishable orientation.
   - Examples: Benzene (C_6H_6) has a C_6 rotation axis passing through the center of the ring.

3. **Improper Rotation Axis (S_n)**:
   - An improper rotation axis combines rotation by a certain angle with a reflection in a plane perpendicular to the axis.
   - Look for rotations combined with a mirror plane perpendicular to the axis.

- Examples: Water (H_2O) has an S_2 improper rotation axis, combining a 180° rotation with a reflection through the plane containing the two hydrogen atoms.

4. **Center of Inversion (i)**:
   - A center of inversion is a point in the molecule where every atom has an equivalent atom on the opposite side, maintaining the same distance.
   - Identify if the molecule has a point where every atom has an equivalent atom at the same distance but opposite in direction.
   - Examples: Benzene (C_6H_6) has a center of inversion at its center.

5. **Rotational-reflection Axis (S_n)**:
   - This combines rotation about an axis with a reflection perpendicular to that axis.
   - Look for an axis where rotation followed by reflection leaves the molecule unchanged.
   - Example: A chair conformation of cyclohexane has a combination of rotation-reflection symmetry.

6. **Helical Symmetry (n-fold screw axis)**:
   - Helical symmetry combines translation along an axis with rotation about the axis.
   - Identify if the molecule has a repeating pattern along a helical path with rotational symmetry.
   - Examples: DNA molecules often exhibit helical symmetry.

Identifying these symmetry elements can provide insights into molecular structure, reactivity, and physical properties. Molecular modelling software or diagrams can also aid in visualizing these elements effectively.

1. *Flow Chart for identifying the Point group:*

Molecular Structure

Is the molecule linear? — Yes → Does the molecule contain an inversion center? — Yes → $D_{\infty h}$
— No → $C_{\infty v}$

Is the molecule linear? — No →

Does the molecule contain two or more unique C_3 axes? — Yes → Does the molecule contain two or more unique C_5 axes? — Yes → Does the molecule contain an inversion center? — Yes → I_h
— No → I

Does the molecule contain two or more unique C_5 axes? — No → Does the molecule contain two or more unique C_4 axes? — Yes → Does the molecule contain an inversion center? — Yes → O_h
— No → O

Does the molecule contain two or more unique C_4 axes? — No → Does the molecule contain one or more reflection planes? — Yes → Does the molecule contain an inversion center? — Yes → T_h
— No → T_d

Does the molecule contain one or more reflection planes? — No → T

Does the molecule contain a proper rotation axis (C_n)? — Yes → Identify the highest order C_n. Are there n perpendicular C_2 axes? — Yes → Does the molecule contain a horizontal reflection plane (σ_h)? — Yes → D_{nh}
— No → Does the molecule contain n dihedral reflection planes (σ_d)? — Yes → D_{nd}
— No → D_n

Identify the highest order C_n. Are there n perpendicular C_2 axes? — No → Does the molecule contain a horizontal reflection plane (σ_h)? — Yes → C_{nh}
— No → Does the molecule contain n vertical reflection planes (σ_v)? — Yes → C_{nv}
— No → Does the molecule contain a $2n$-fold improper rotation axis? — Yes → S_{2n}
— No → C_n

Does the molecule contain a proper rotation axis (C_n)? — No → Does the molecule contain a reflection plane? — Yes → C_s
— No → Does the molecule contain an inversion center? — Yes → C_i
— No → C_1

2. Procedure for Drawing/importing 3D structure and predicting point groups

- The 3D structures of the molecules can be drawn using model kit menu or we can import it from database
- In this study we have imported the structures from database using the option get MOL in file menu

2.1. Steps for importing structure from database:

- Open Jmol interface
- Click on the file menu
- Select Get MOL option
- A dialogue box opens
- Type the name of the molecule to be downloaded
- The 3D structure of the molecule will be displayed on the Jmol interface
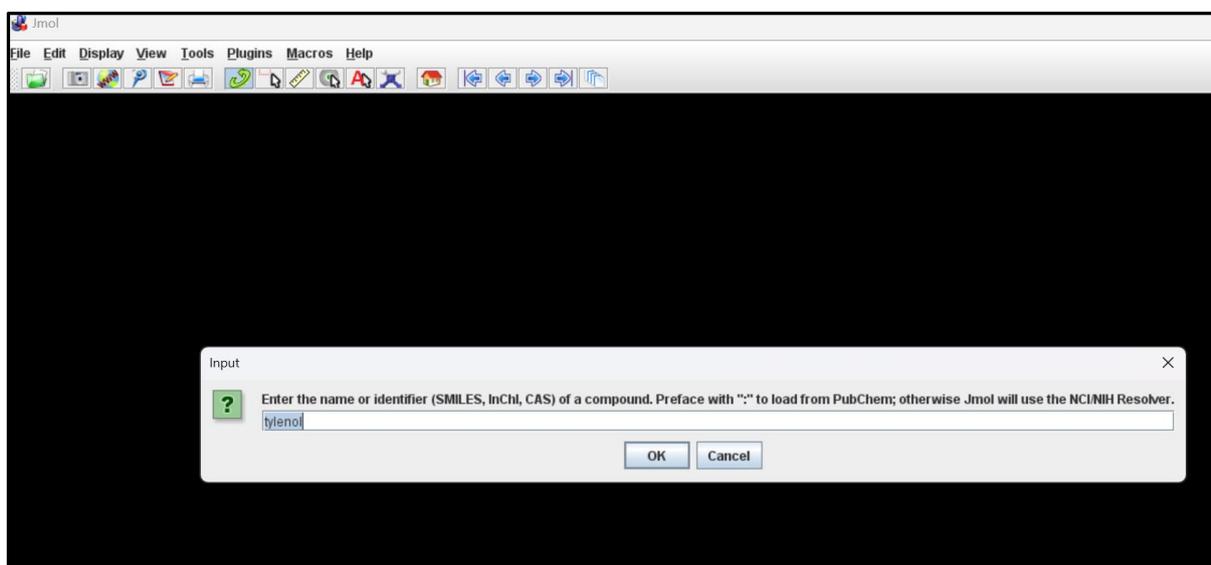
2.2. Predicting the point group using script commands

- Click the file menu
- Select the option Console…
- The dialogue box opens
- Now type the script command "**$ draw pointgroup**" and press enter
- The point group of the molecule is displayed

3. *Check Against Examples:*

3.1. Example 1: Ethylene
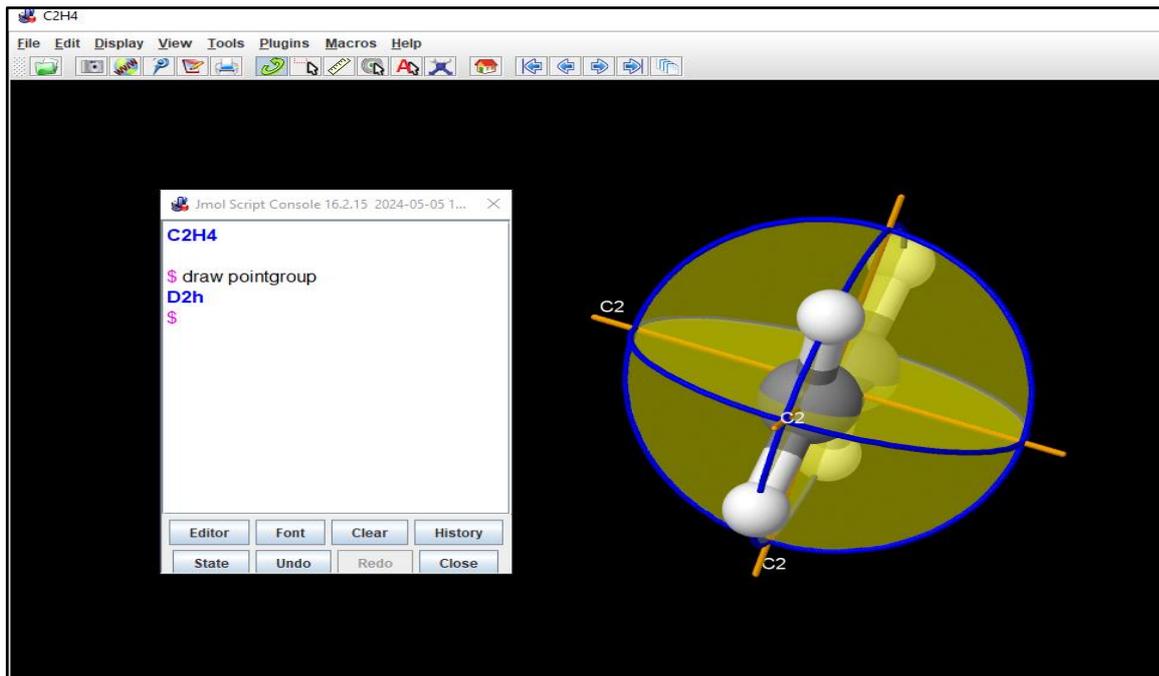
Non axial (C_1, C_i, C_s)

Step1: Molecular geometry

- Non- Linear

Step 2: Details of rotation

- The molecule does not contain rotation axis

Step3: Details of reflection plane

- The molecule contains reflection plane

Step4: Details of C_3 axes

- The molecule does not contain C_3 axes

Step5: Molecule point group

- D_{2h}

3.2. Examples of Linear Molecules:

3.2.1. Carbon dioxide
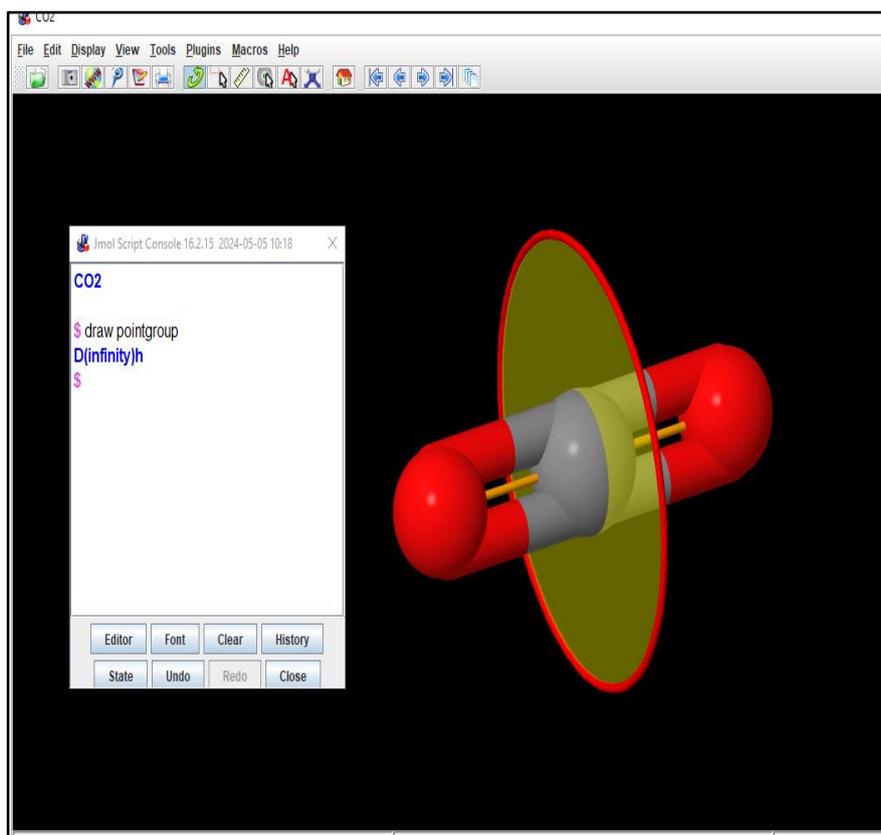
Step1: Molecule geometry

- Linear

Step2: Rotation axis

- Infinite rotation axis (C infinite)

Step3:Inversion center

- The molecules contains inversion center

Step4: Molecule point group

- D∞h

3.2.3. Acetylene (Linear)
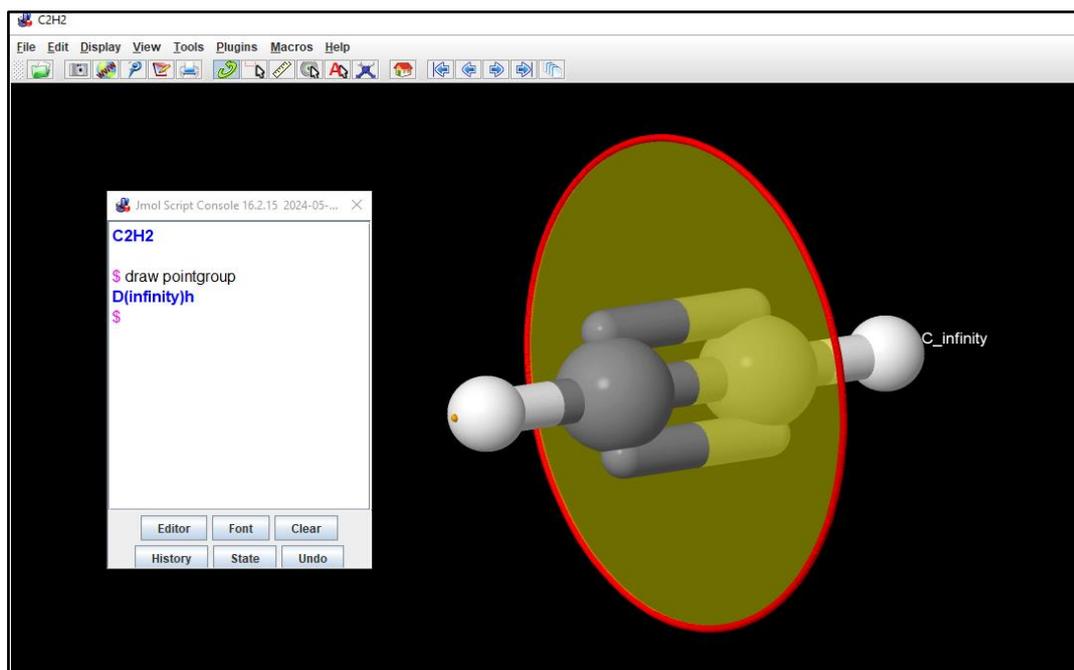
Step1: Molecule geometry

- Linear

Step2: Rotation axis

- Infinite rotation axis

Step3:Inversion center

- This molecule contains inversion center

Step4: Molecule point group

- D∞h

3.2.4. Hydrogen cyanide (Linear)
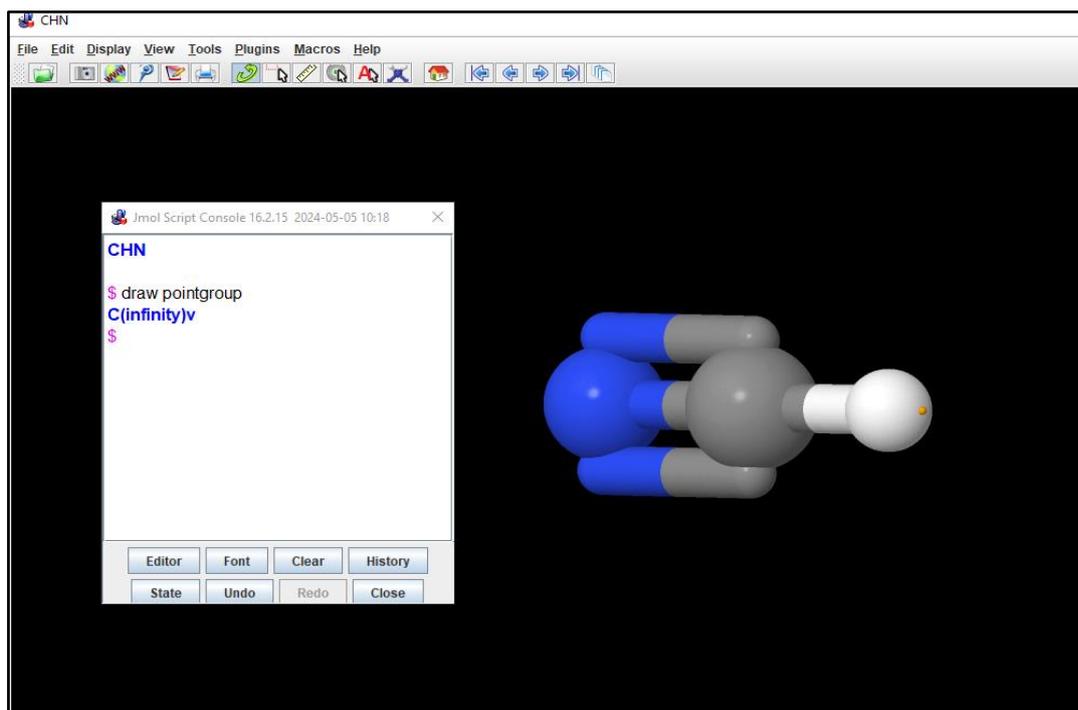
Step1: Molecule geometry

- Linear

Step2: Rotation axis

- Infinite rotation axis (Cinfinite)

Step3: Inversion center

- This molecule does not contain inversion center

Step4: Molecule point group

- $C\infty_v$

3.3. Hydrogen peroxide (Non- linear)
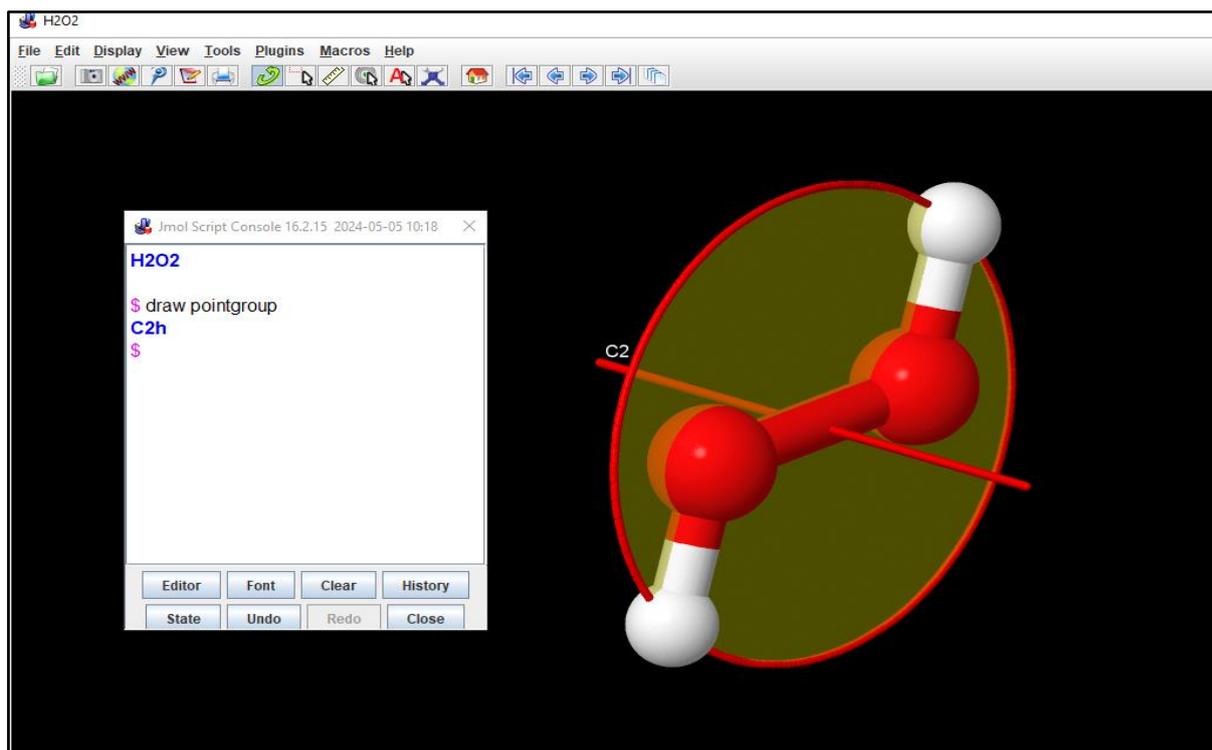
Cyclic (C$_n$)

step1: Molecule geometry

- Non -linear

Step2: Rotation axis (C$_n$)

- Molecule contains a C$_2$ axis passing through on two oxygen atom

Step3: Details of C$_3$ axis

- This molecule does not contains any C$_3$ axis

Step4: Details of vertical and reflection plane

- This molecule does not contains reflection and vertical plane

Step5: Molecule point group

- C$_2$

3.4. **Twistane (Non- linear)**
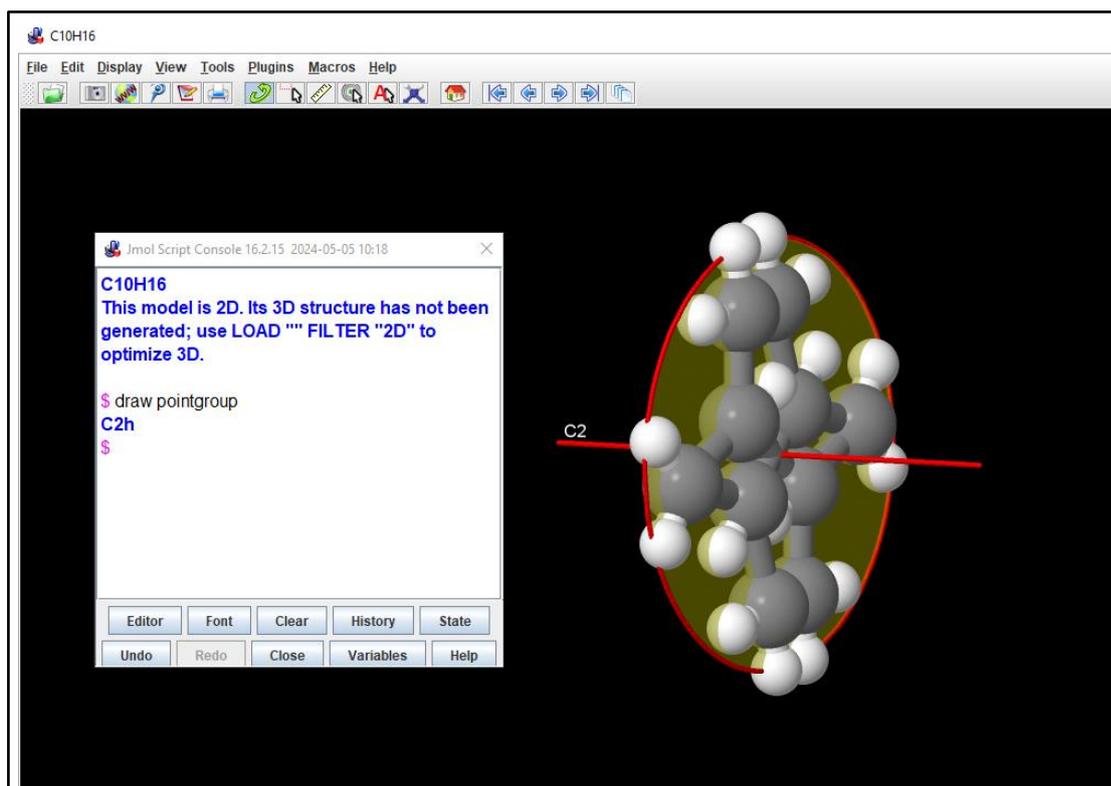
Dihedral (D_n)

Step1: Molecule geometry

- Non -linear

Step2: Details of rotation axis

- 2 C_2 axes perpendicular to a C_2 axes

Step3: Details of C_3 axis

- This molecule does not contains unique C_3 axes

Step4: Details of vertical and reflection plane

- This molecule does not contains vertical and reflection plane

Step5: Molecule point group

- C_{2h}

3.5. Water (Non- linear)
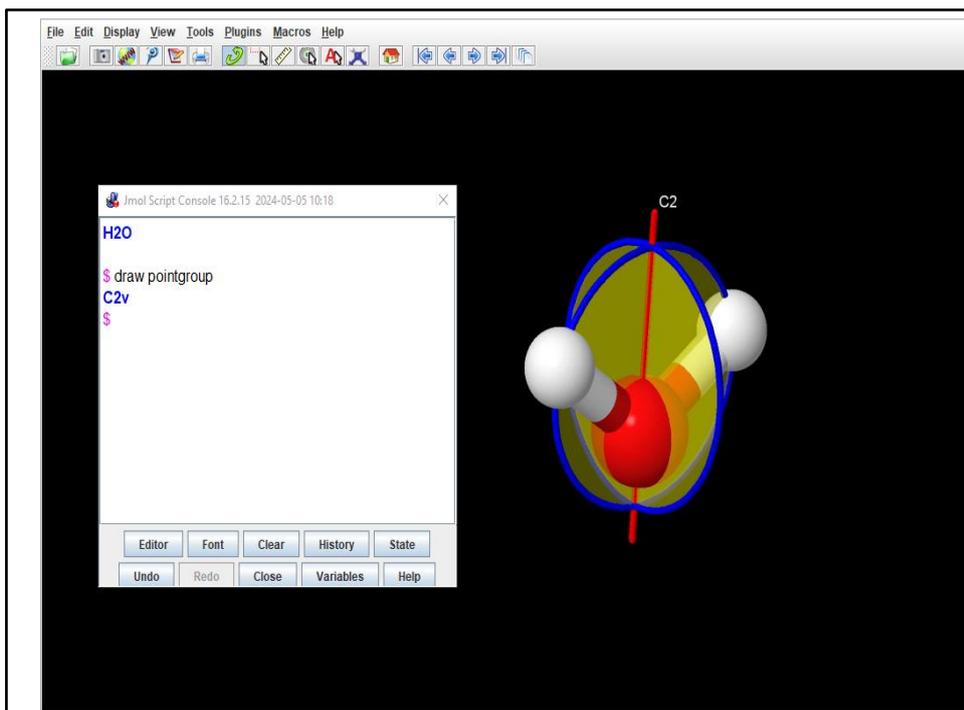
Pyramidal (C$_{nv}$)

Steps1: Molecule geometry

- Non -linear

Step2: Proper rotation axis (C$_n$)

- C$_2$ axis passing through the oxygen atom

Step3: Details of vertical reflection plane

- This molecule contains 2 vertical reflection plane

Step4: Horizontal reflection plane

- Not contains reflection plane

step5:Details of unique C$_3$ axes

- This molecule not contain C$_3$ axes

Step 5: Molecule point group

- C$_{2v}$

3.6. Benzene 1,3,5 triol (Non- linear)
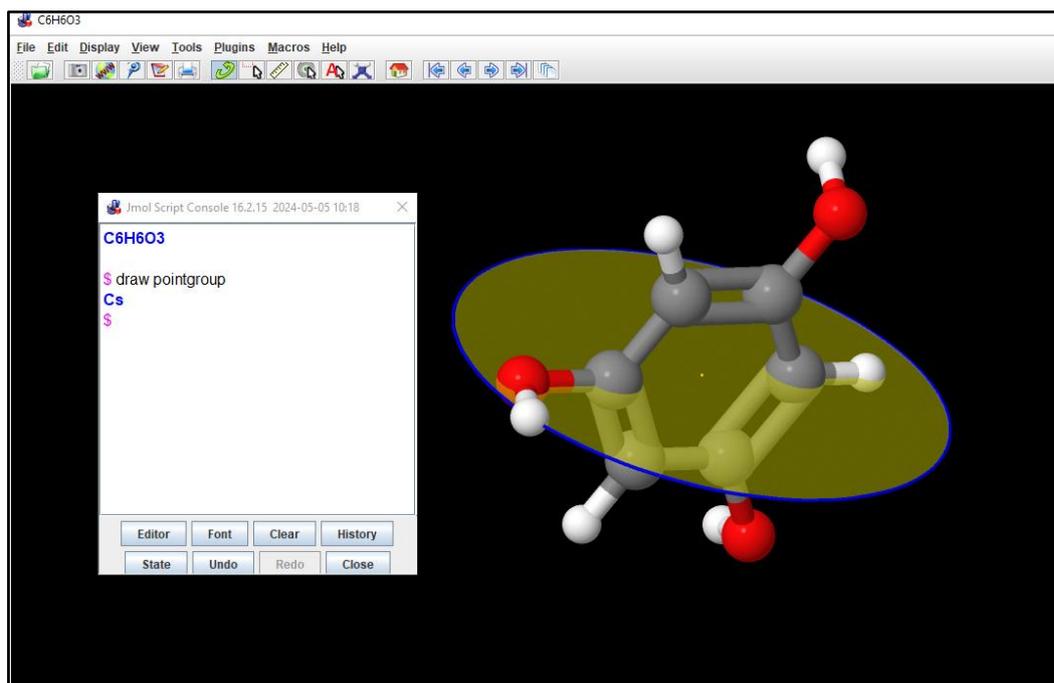
Reflection (C$_{nh}$)

Step1: Molecule geometry

- Non -linear

Step2: No.of unique C$_3$ axes

- One unique C$_3$ axes

Step3: Details of horizontal reflection plane

- Molecule contains horizontal reflection plane

Step4: Details of highest -order proper rotation axis

- 3-fold axis

Step5: Molecule point group

- C$_{3h}$

3.7. Diborane (Non- linear)
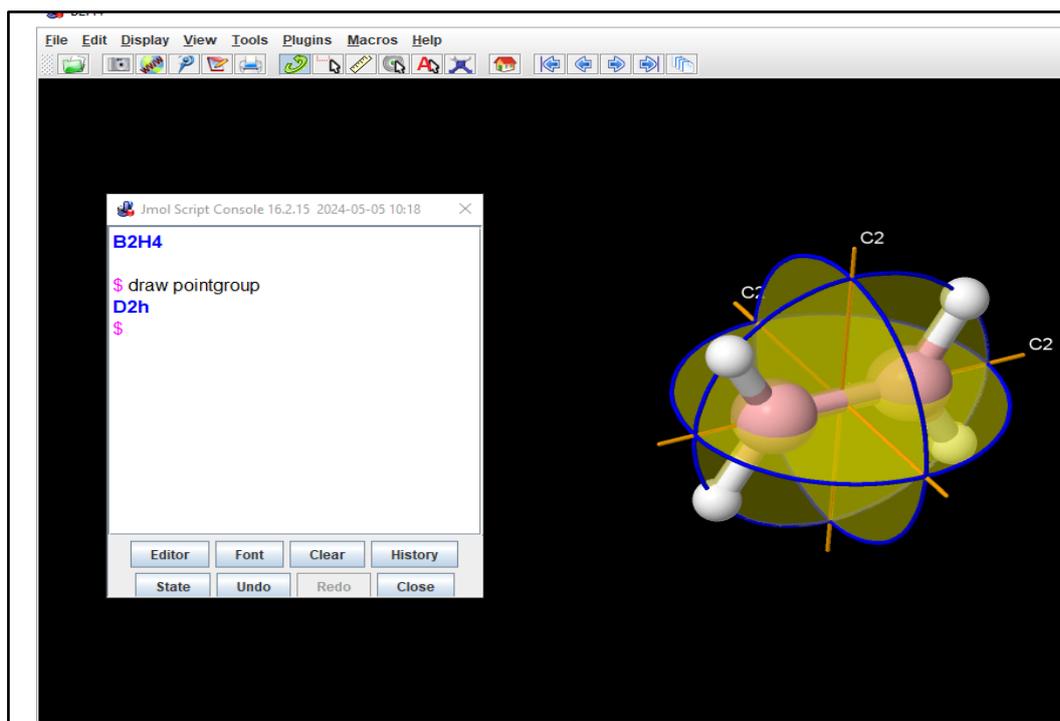
Prismatic (D_nh)

Step1: Molecule geometry

- Non -linear

Step2: Rotation axis

- C_2 axes passing through the boron atom

Step3: Details of unique C_2 axis

- The molecule not contains C_3 axis

Step4: Details of highest order proper axis

- Highest order proper axis is 2-fols axis

Step5: Horizontal reflection plane

- The molecule contains horizondal reflection plane

Step6: Molecule point group

- D_{2h}

3.8. **Allene (Non- linear)**
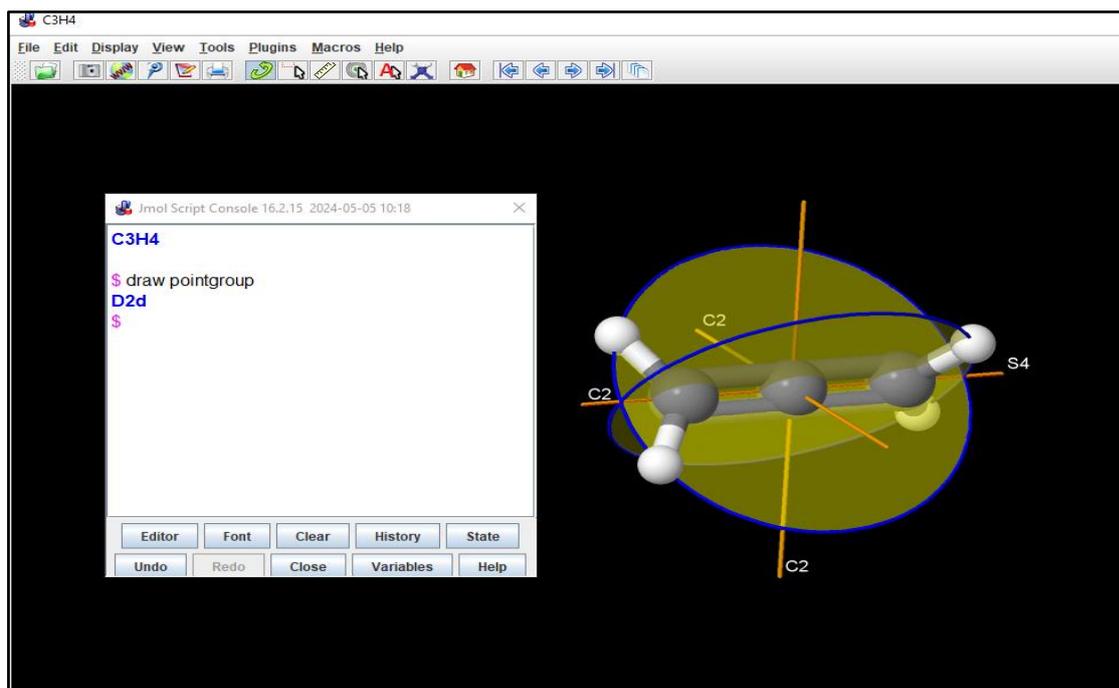
Anti-prismatic (D$_{nd}$)

Step1: Molecule geometry

- Non-linear

Step2: Rotation axis

- 2 C$_2$ axis perpendicular to a C$_2$ axis

Step3: Unique C$_3$ axis

- This molecule not contains any C3 axis

Step4: Dihedral reflection plane

- Contains 2 dihedral reflection plane

Step5: Molecule point group

- D$_{2d}$

3.9. Tetrabromoneopentane (Non- linear)
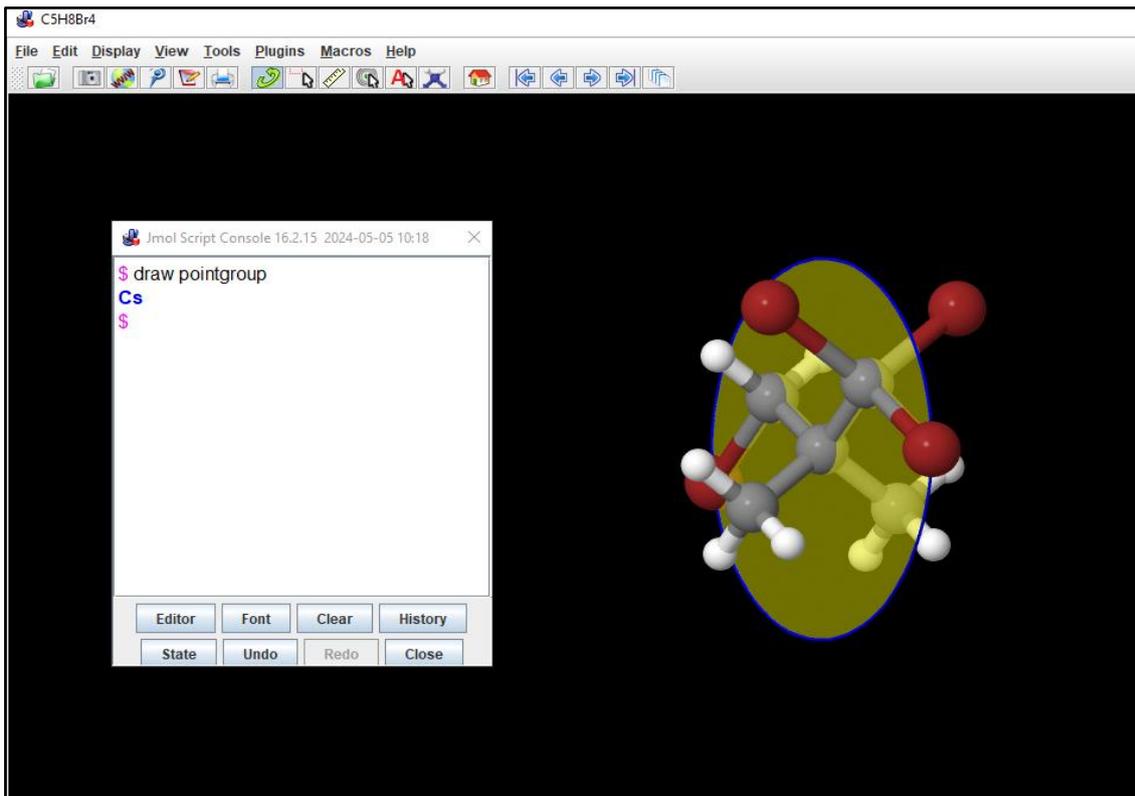
Improper rotation axis (S_n)

Step 1:Molecule geometry

- Non-linear

Step2:Details of improper rotation axis

- The molecule contains S_4 rotation axis

Step3: Details of rotation axis

- Contains C_2 axis

Step4: Details of vertical and horizontal reflection plane

- Not contains both of plane

Step5: Molecule point group

- S_4

3.10. **Methane (Non- linear)**
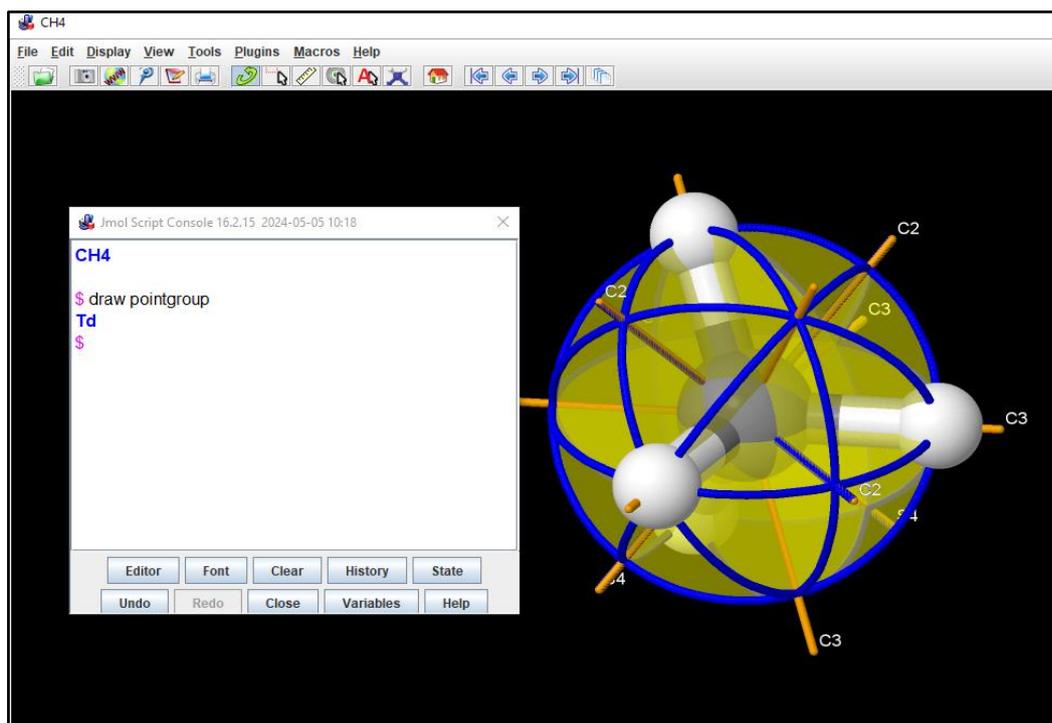
Tetrahedral (T,Th,Td)

Step1: Molecule geometry

- Non-linear

Step2: Proper rotation axis

- 2 C_2 axis

Step3: No.of unique C_3 axis

- Contains 4 unique C_3 axis

Step4: Details of reflection plane

- The molecule contains 6 reflection plane

Step5: Molecule point group

- T_d

3.11. Sulphur hexafluoride
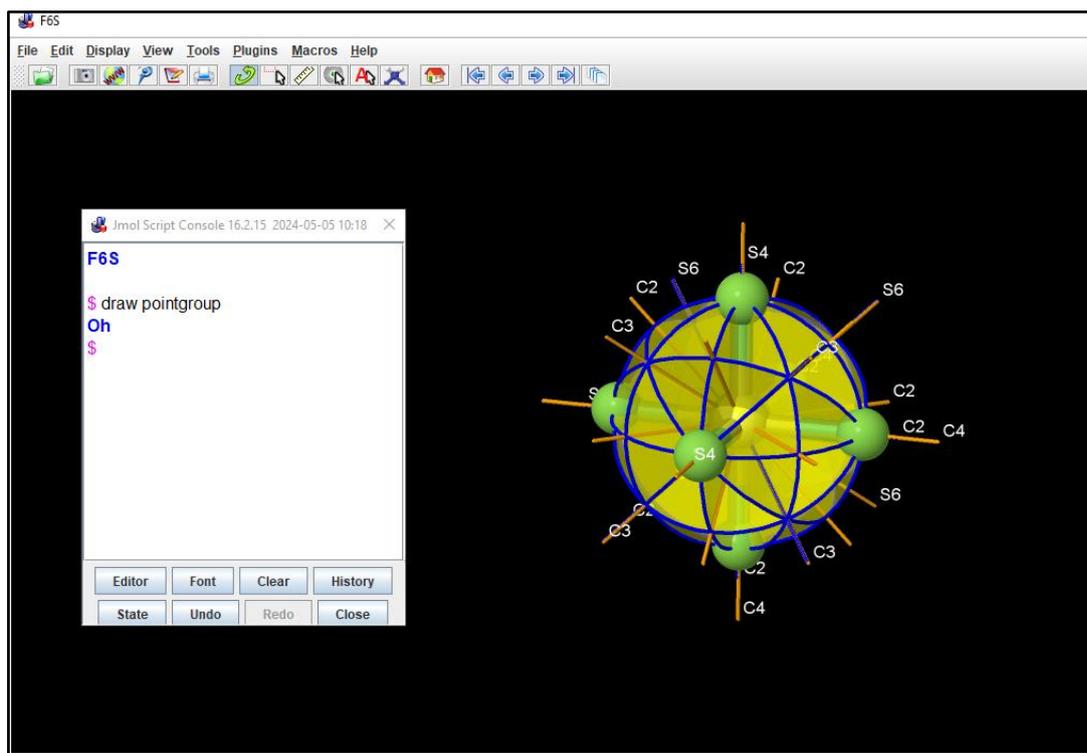
Octahedral (O,Oh)

Step1: Molecule geometry

- Non-linear

Step2: No.of C_3 axis

- 4 C_3 axis

Step3: No.of C_4 axis

- 3 C_4 axis

Step 4: Inversion center

- This molecule contains inversion center

Step5: Molecule point group

- O_h

Conclusion

Jmol is a highly effective tool for learning point groups in the context of molecular symmetry and crystallography. Its interactive 3D visualization capabilities allow students and researchers to explore and manipulate molecular structures, providing an intuitive and engaging way to

understand complex symmetry operations. By offering real-time rotation, reflection, and inversion of molecular models, Jmol enhances spatial reasoning skills and deepens comprehension of abstract symmetry concepts.

Moreover, Jmol's accessibility as a free, open-source application ensures that it is readily available to a wide audience, including educators and students at various educational levels. Its integration with online resources and ease of use make it a versatile addition to both classroom settings and independent study. By facilitating a hands-on approach to learning, Jmol not only aids in grasping theoretical aspects of point groups but also prepares users for practical applications in fields such as chemistry, materials science, and molecular biology.

Overall, the use of Jmol in studying point groups exemplifies the positive impact of interactive technology on education, fostering a more comprehensive and engaging learning experience.