

Predicting the point group of molecules using Jmol application

M.Nivetha¹, P.Sivaranjana²

¹*Department of Chemistry, Kaliswari college of arts and science, Sivakasi- 626123*

²*Department of Chemistry, Kalasalingam Academy of Research and Education- 626126*

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 molecules 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 molecules offers a better platform for understanding the concept of symmetry and point group of various molecules. 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 molecules as example for each point group.

Keywords

Point group, symmetry, rotation, axis

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. During my internship, I worked on a project 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 and easy to use, 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.

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 internship 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 $(360^\circ/n)$ 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 S_2 operation involves a 180° 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° around its central axis.

2. D_n : Molecules with an n -fold rotation axis and n perpendicular C_2 axes. For example, ethane (C_2H_6) in its staggered conformation belongs to the D_{3d} 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 C_i 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.

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.

1. 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 ($360^\circ/n$) 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):**

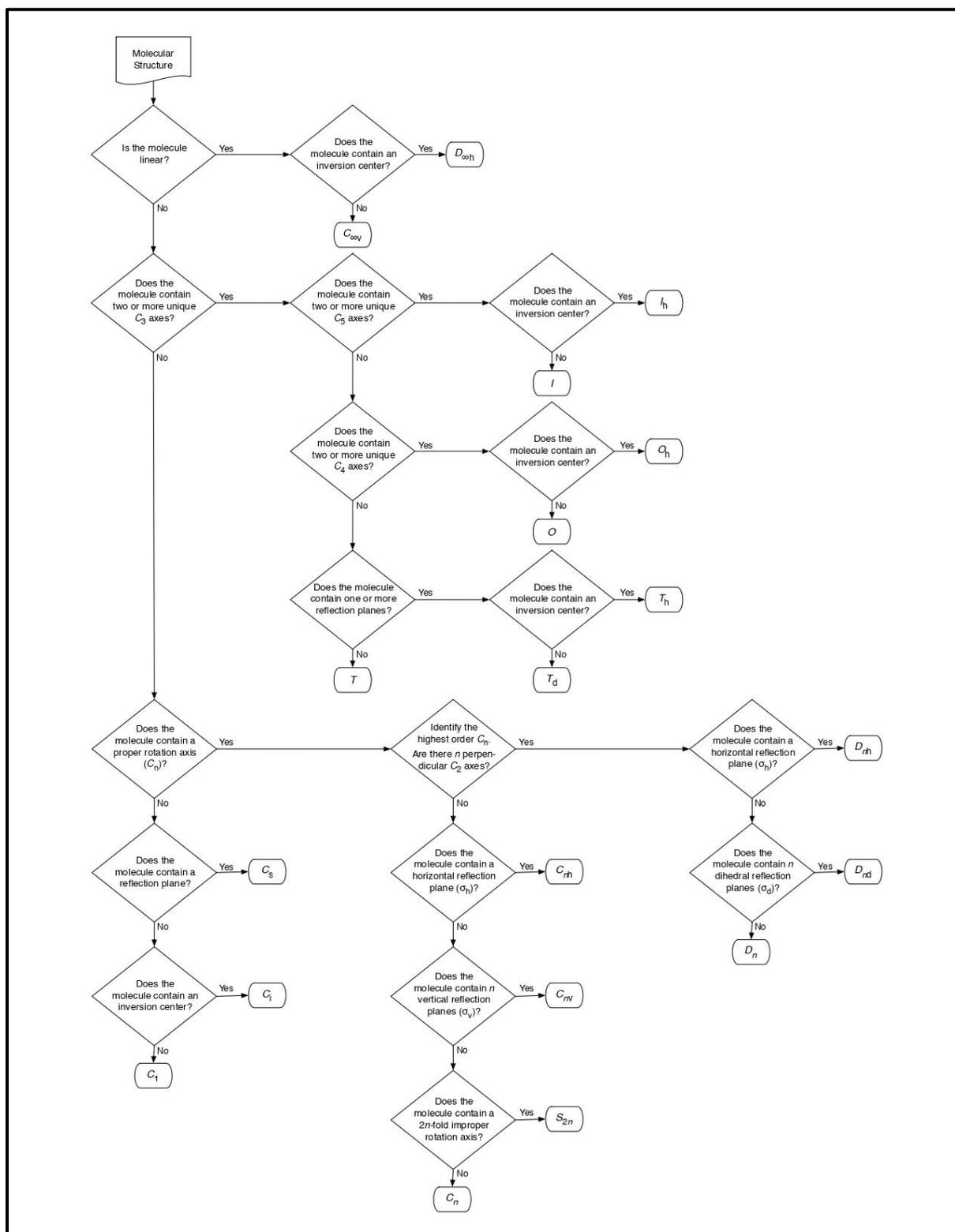
- This combines rotation about an axis with a reflection perpendicular to that axis.
- Look for an axis where rotation followed by reflection leaves the molecule unchanged.
- Example: A chair conformation of cyclohexane has a combination of rotation-reflection symmetry.

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.

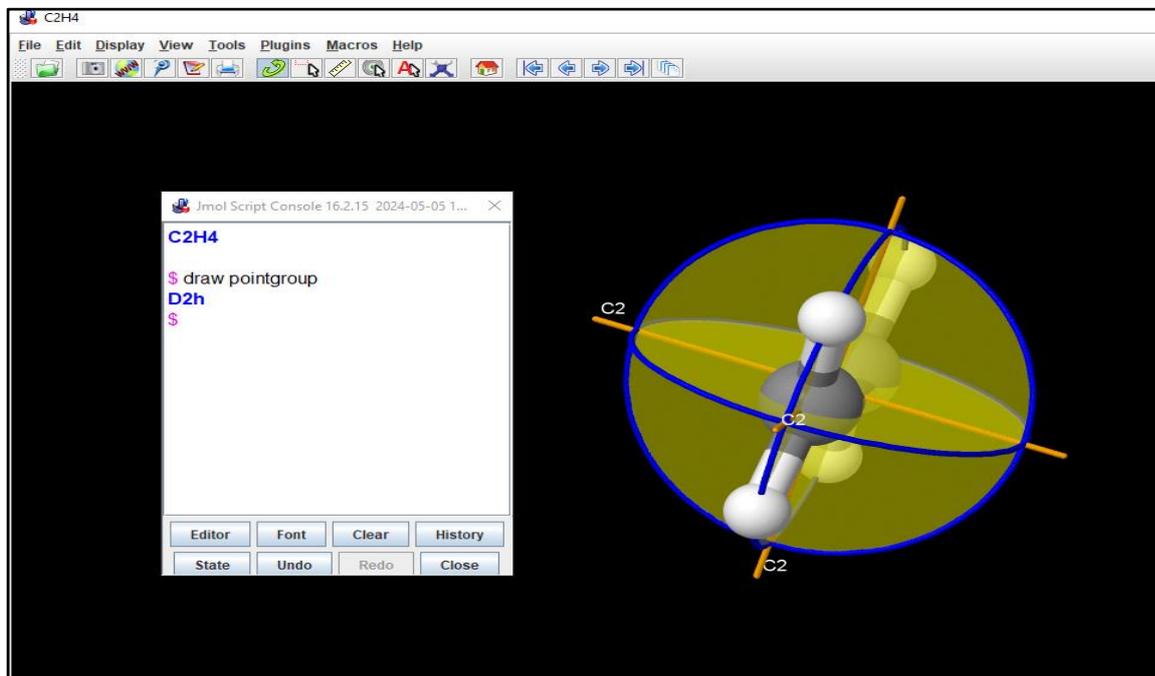
2. Flow Chart for identifying the Point group:



(Ref. <http://faculty.otterbein.edu/djohnston/sym/challenge/index.html>)

3. Check Against Examples:

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 contains rotation axis

Step3: Details of reflection plane

- The molecule contains reflection plane

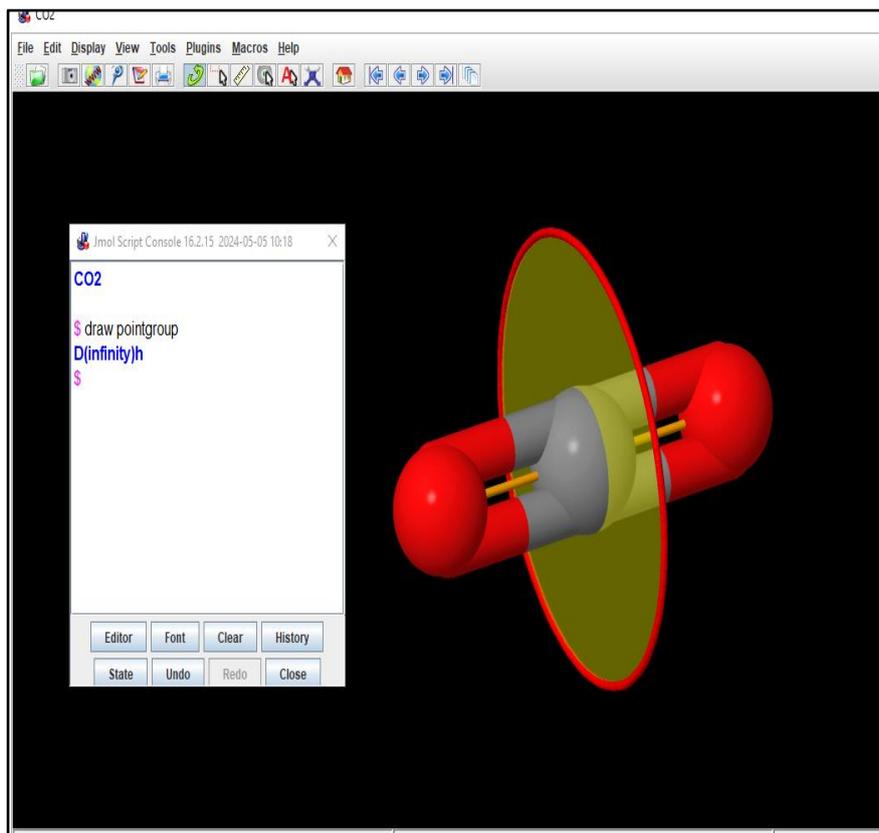
Step4: Details of C_3 axes

- The molecule does not contain C_3 axes

Step5: Molecule point group

- D_{2h}

Examples of Linear Molecules:



1. carbon dioxide

Step1: Molecule geometry

- Linear

Step2: Rotation axis

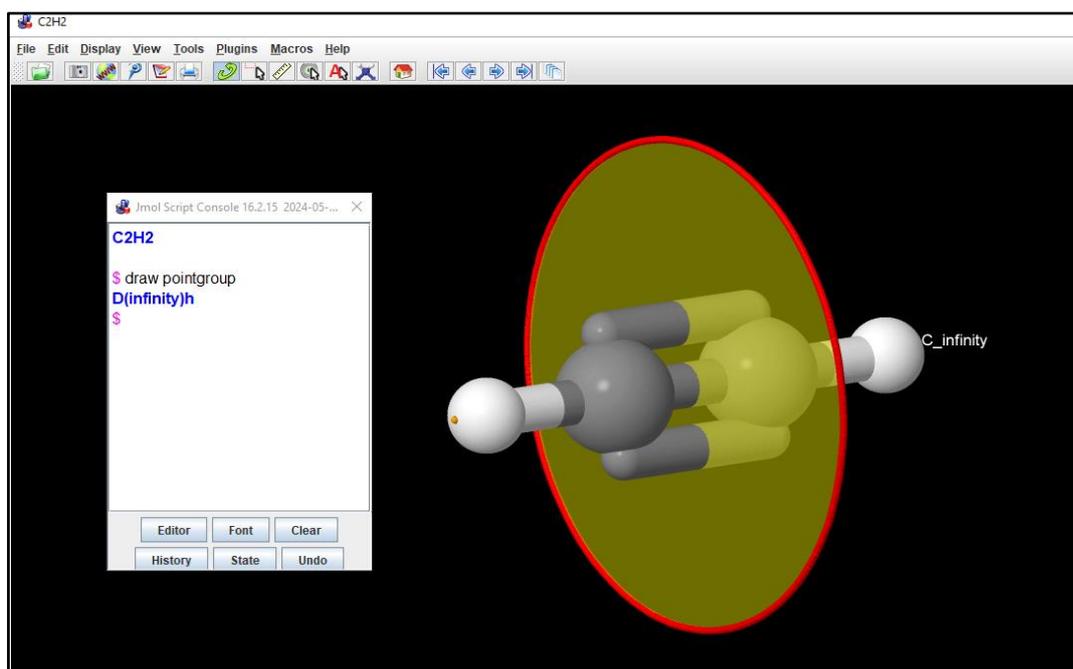
- Infinite rotation axis (C infinite)

Step3: Inversion center

- The molecule contains an inversion center

Step4: Molecule point group

- D_{∞h}



2.Acetylene

Step1: Molecule geometry

- Linear

Step2: Rotation axis

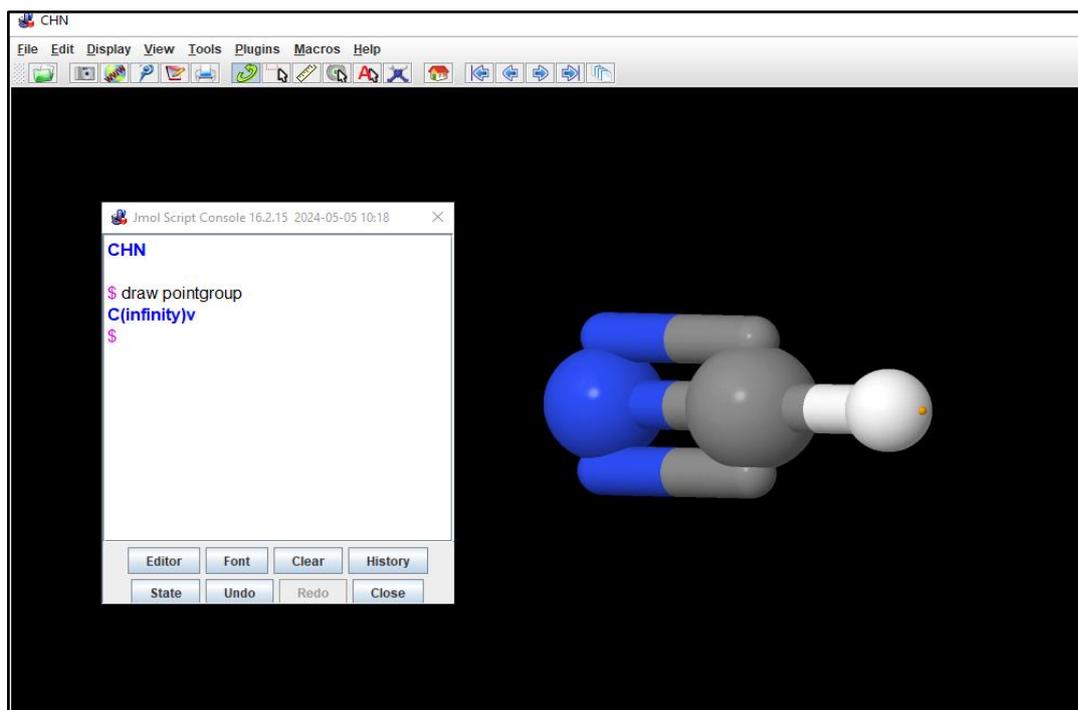
- Infinite rotation axis

Step3: Inversion center

- This molecule contains inversion center

Step4: Molecule point group

- $D_{\infty h}$



3. Hydrogen cyanide

Step1: Molecule geometry

- Linear

Step2: Rotation axis

- Infinite rotation axis (C_{∞})

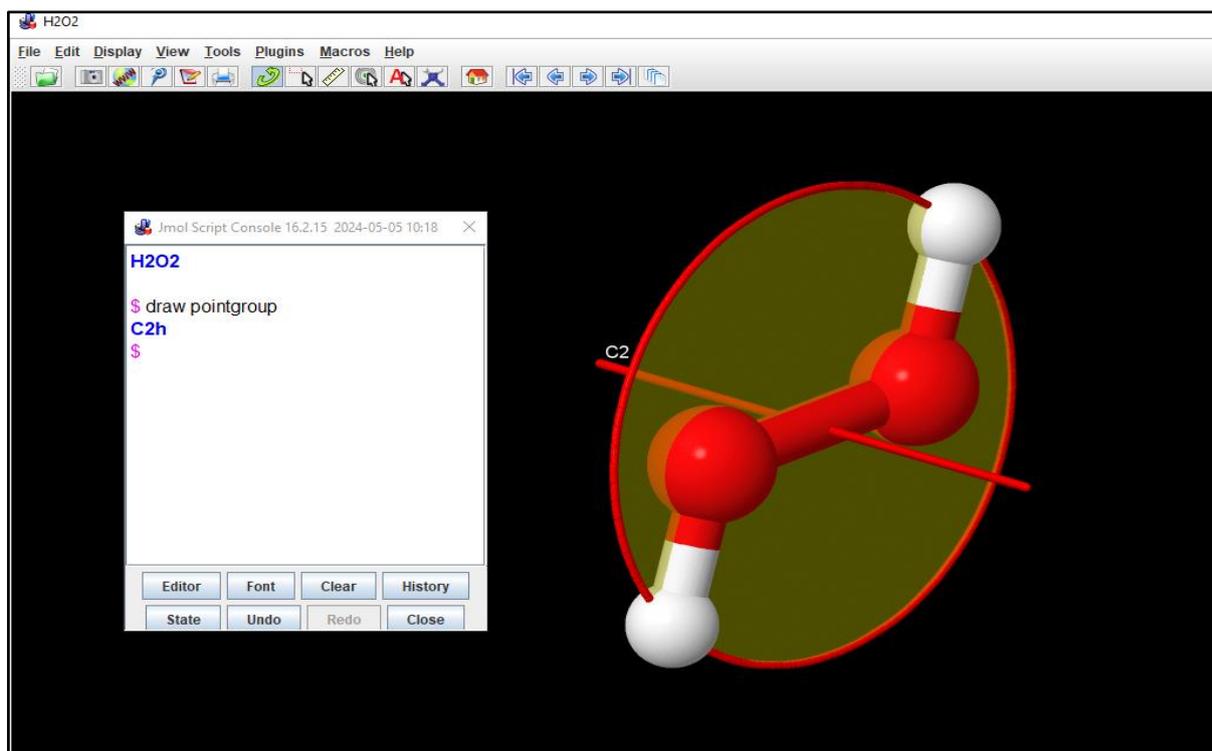
Step3: Inversion center

- This molecule does not contain an inversion center

Step4: Molecule point group

- $C_{\infty v}$

Example 3 : Hydrogen peroxide



Cyclic (C_n)

step1: Molecule geometry

- Non -linear

Step2: Rotation axis (C_n)

- Molecule contains a C₂ axis passing through on two oxygen atom

Step3: Details of C₃ axis

- This molecule does not contains any C₃ axis

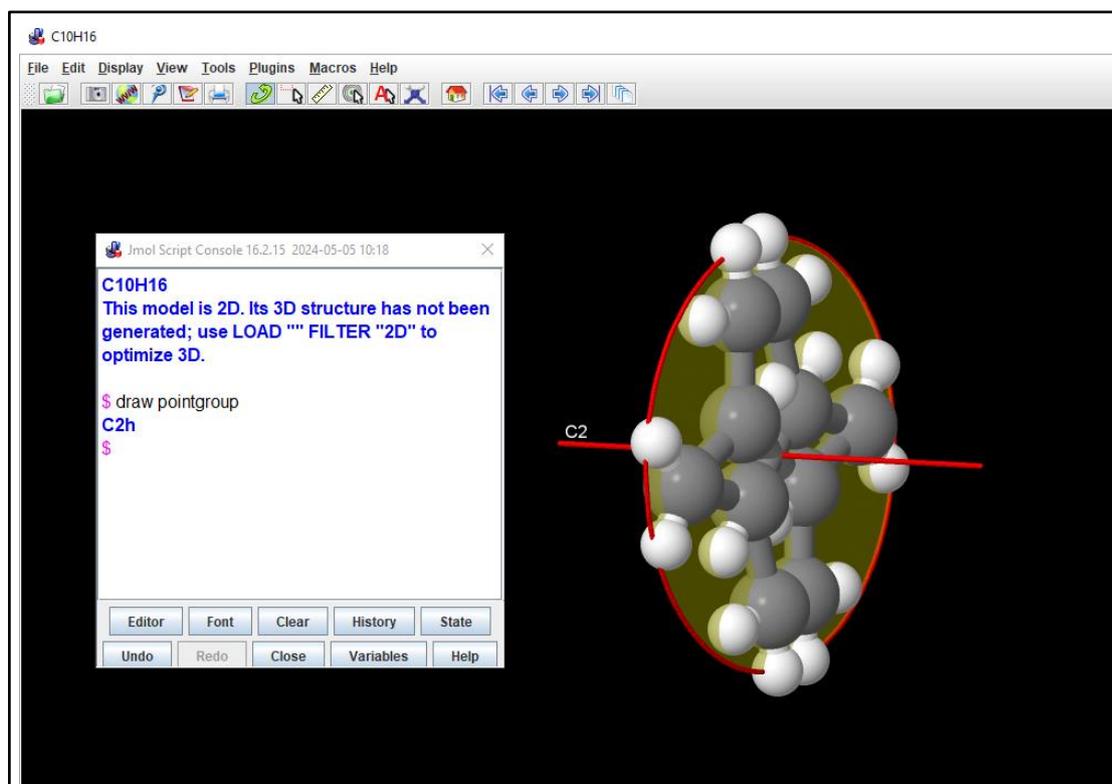
Step4: Details of vertical and reflection plane

- This molecule does not contains reflection and vertical plane

Step5: Molecule point group

- C₂

Example 4 : Twistane



Dihedral (D_n)

Step1: Molecule geometry

- Non-linear

Step2: Details of rotation axis

- 2 C₂ axes perpendicular to a C₂ axes

Step3: Details of C₃ axis

- This molecule does not contains unique C₃ axes

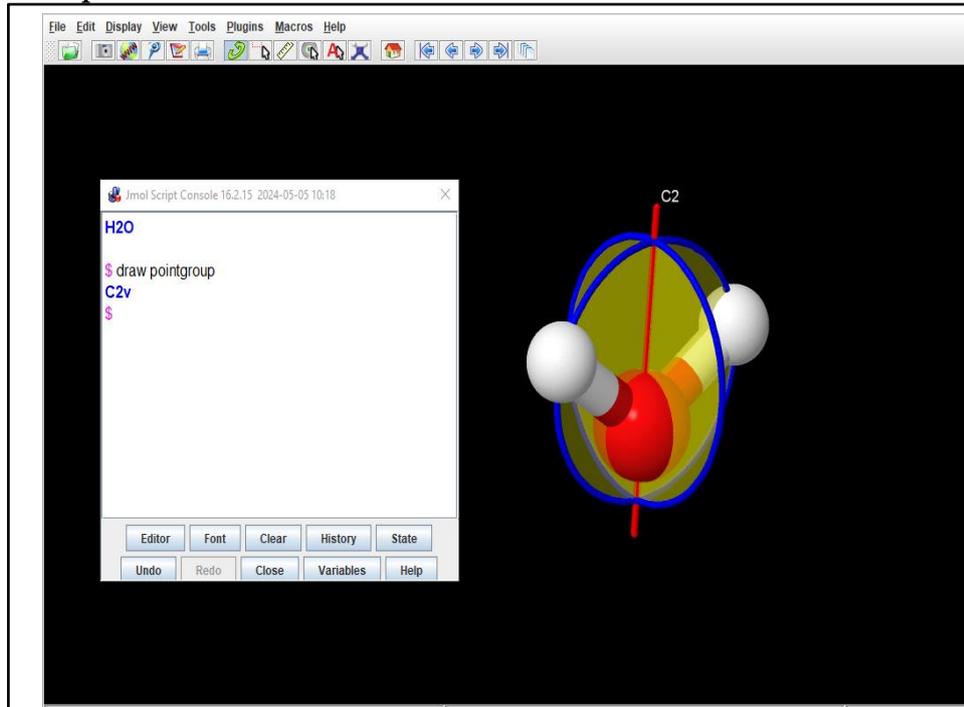
Step4: Details of vertical and reflection plane

- This molecule does not contains vertical and reflection plane

Step5: Molecule point group

- C_{2h}

Example 5 : Water



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

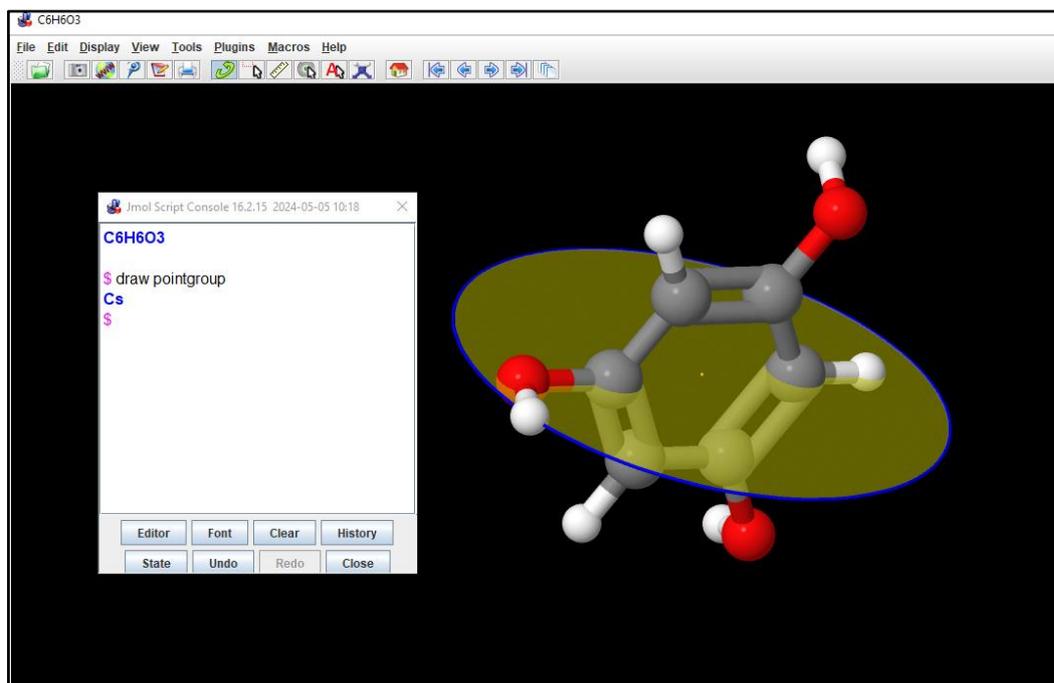
step5:Details of unique C_3 axes

- This molecule not contains C_3 axes

Step 5: Molecule point group

- C_{2v}

Example 6 : Benzene 1,3,5 triol



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

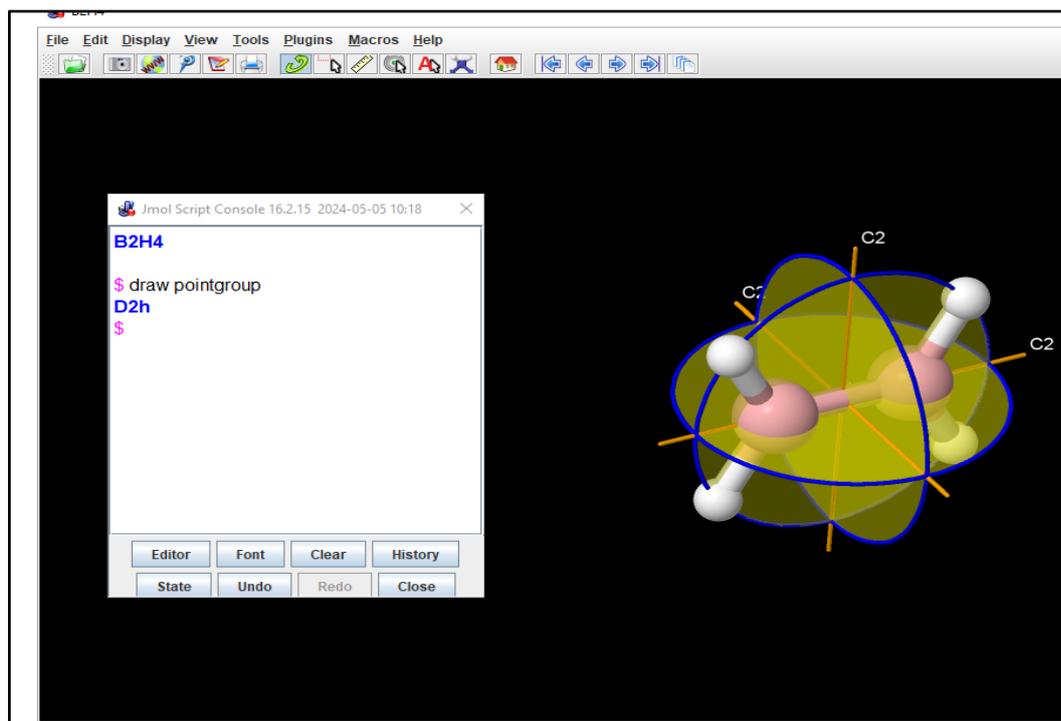
Step4: Details of highest -order proper rotation axis

- 3-fold axis

Step5: Molecule point group

- C_{3h}

Example 7 : Diborane



Prismatic (D_{nh})

Step1: Molecule geometry

- Non-linear

Step2: Rotation axis

- C₂ axes passing through the boron atom

Step3: Details of unique C₂ axis

- The molecule not contains C₃ axis

Step4: Details of highest order proper axis

- Highest order proper axis is 2-fols axis

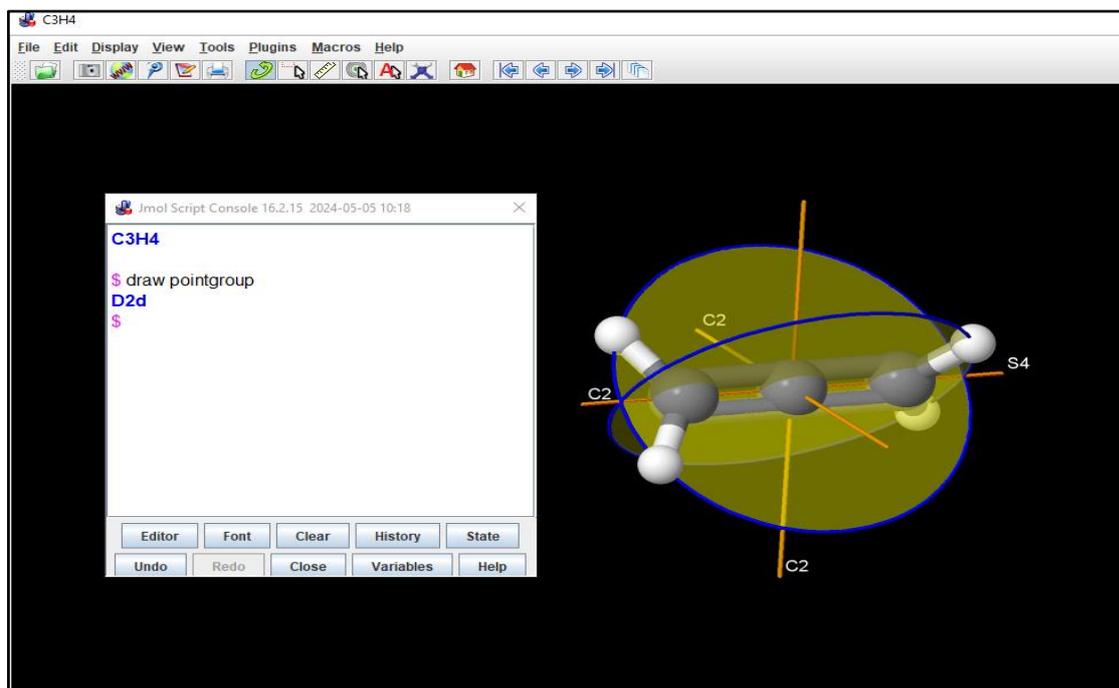
Step5: Horizontal reflection plane

- The molecule contains horizonsdal reflection plane

Step6: Molecule point group

- D_{2h}

Example 8 : Allene



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 C_3 axis

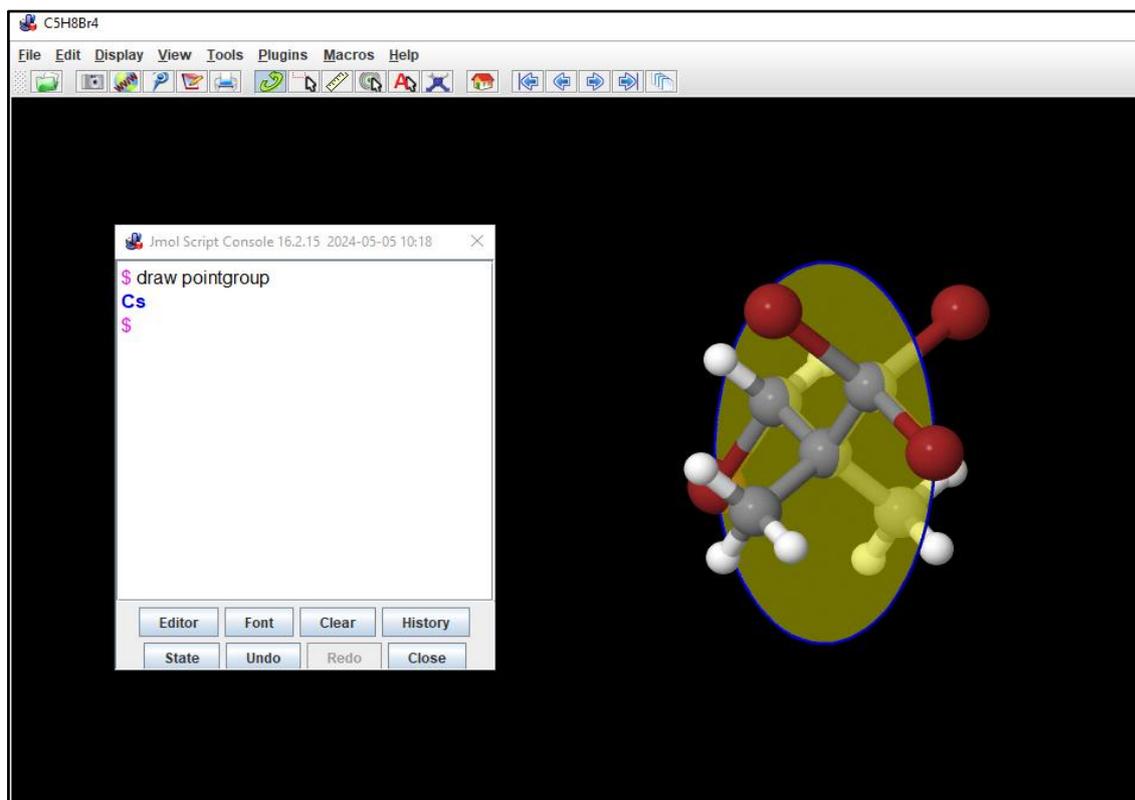
Step4: Dihedral reflection plane

- Contains 2 dihedral reflection plane

Step5: Molecule point group

- D_{2d}

Example 9 : Tetrabromoneopentane



Improper rotation axis (S_n)

Step 1: Molecule geometry

- Non-linear

Step 2: Details of improper rotation axis

- The molecule contains S_4 rotation axis

Step 3: Details of rotation axis

- Contains C_2 axis

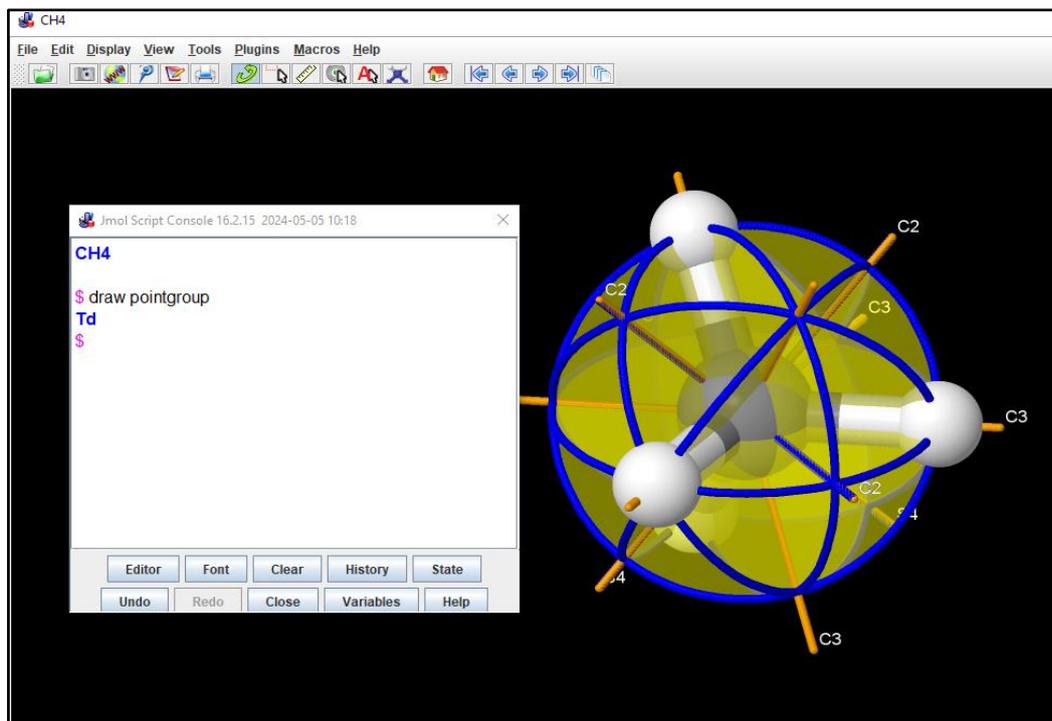
Step 4: Details of vertical and horizontal reflection plane

- Not contains both of plane

Step 5: Molecule point group

- S_4

Example 10 : Methane



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

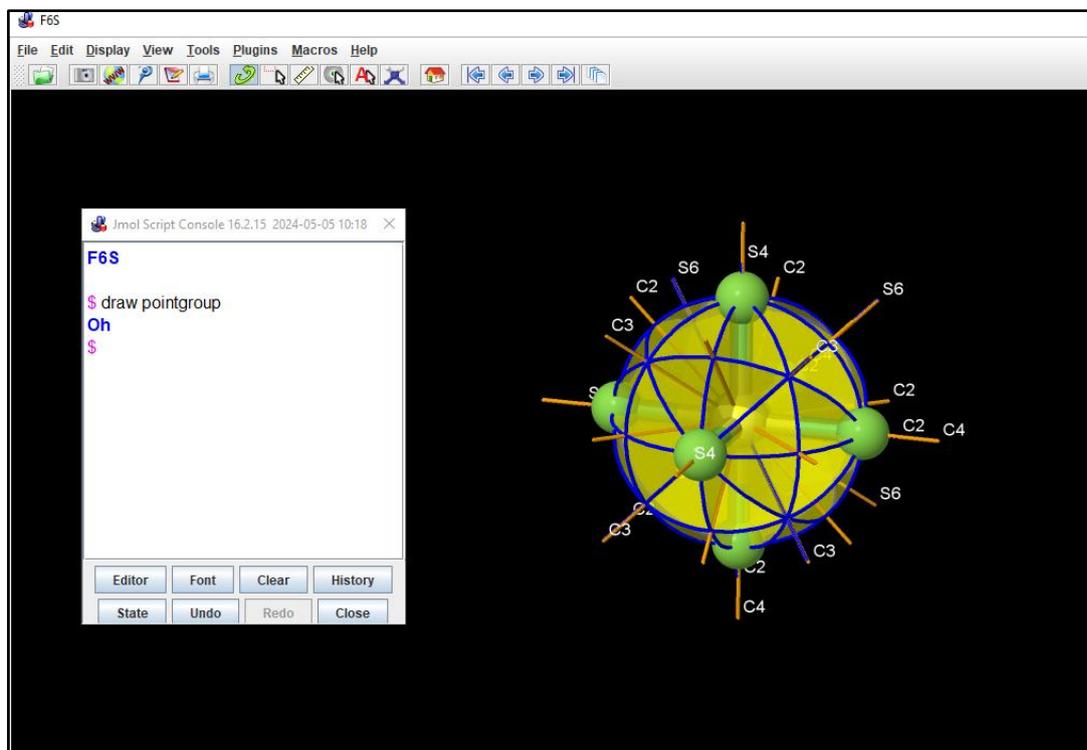
Step4: Details of reflection plane

- The molecule contains 6 reflection plane

Step5: Molecule point group

- T_d

Example 11 : Sulphur hexafluoride



Octahedral (O,Oh)

Step1: Molecule geometry

- Non-linear

Step2: No.of C₃ axis

- 4 C₃ axis

Step3: No.of C₄ axis

- 3 C₄ 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.

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