

## Understanding the Geometry and Shape of Inorganic Molecules

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### Aim and Objectives:

To draw and visualise geometry, bond length and bond angle of simple inorganic molecules.

To monitor the energy change for a molecule with change in bonding elements and analyze their reactivity.

### Introduction:

Inorganic molecules like  $\text{PCl}_3$ ,  $\text{PCl}_5$ ,  $\text{AlCl}_3$ , etc are used as reagents / catalysts in many reactions. These reagents play important roles as Lewis acids, reagent in substitution reactions, etc., Various theories like VBT, VSEPR, etc., are used to explain the shape, geometry and orientation of these of molecules. These theoretical concepts are often complex to explain and students find it difficult to visualise the shapes of molecules. This project will attempt to explain the geometry and shape of the molecules by drawing their 3D representations. It will emphasize the relationship between a lone pair and a bond pair and significance of their contributions to the shape of the molecules. From this understanding, we hope to extend the explanation to coordination complexes as well. This can be applied to explain crystal field splitting of complexes with weak field and strong field ligands in these complexes.

Inorganic chemistry deals with geometry, shape and hybridisation of molecules. There are many existing theories like Octet rule, Lewis dot structure, Valence Bond theory, etc., These theories describe geometry, bond energy, bond length, effect of substituent on the bond length of a molecule, etc., Students find it difficult and boring to remember these theories.

### Octet rule:

<sup>1</sup>The octet rule states that atoms tend to form compounds in ways that give them eight electrons in their outermost orbits or valence shells, and thus satisfying the Octet rule.

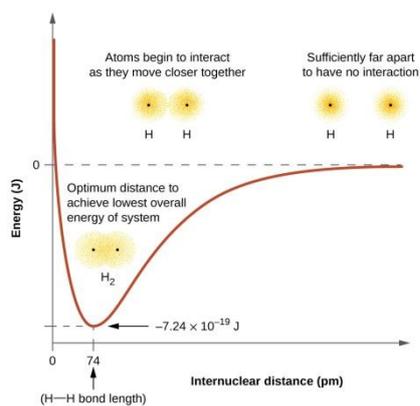
### Valence bond theory:

Atomic orbitals of two different atoms overlap to form a covalent bond.

Each atom contributes one electron to form an electron pair.

VBT describes electrons of each bonding atom are attracted to the nucleus of other bonding atom. This attraction increases till the atom reaches to the minimum distance where the electron density increases and causes repulsion.

As the atom reaches to minimum distances they have low potential energy and it is said that bond is formed between atoms.



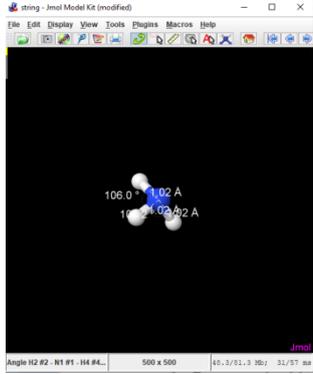
Valence Shell Electron Pair Repulsion theory:

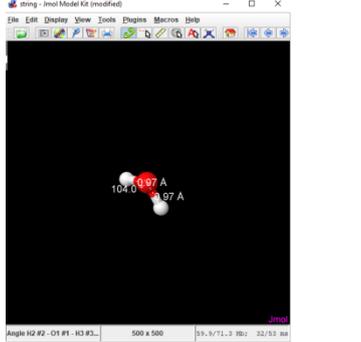
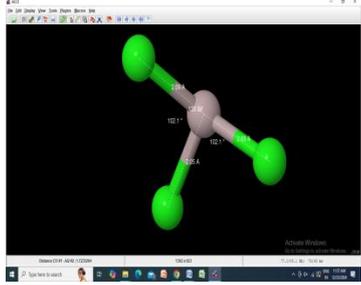
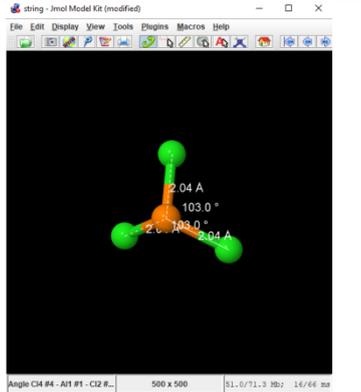
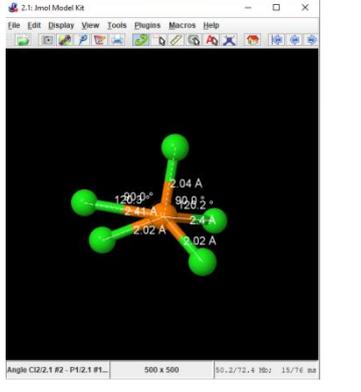
Valence Shell Electron Pair Repulsion Theory (VSEPR) explains about geometry of molecules. It explains the three dimensional orientation of molecules in XYZ plane. This theory considers lone pair and bond pair of electrons in a molecule for predicting the geometry and orientation of a molecule.

Problem:

To measure bond length and bond angle of the following molecules using Jmol Application. Phosphorus trichloride (PCl<sub>3</sub>), Phosphorus pentachloride (PCl<sub>5</sub>), Aluminium chloride (AlCl<sub>3</sub>), Water (H<sub>2</sub>O) and Ammonia (NH<sub>3</sub>)  
To compare the bond angle and bond length with change in species.

Table No.: 1

Sr. No.	Name of Molecule	Image	Parameters from Jmol Application BL (Bond length) BA (Bond Angle) E= Energy
1.	Ammonia (NH <sub>3</sub> )	 <p>The screenshot shows the Jmol application window with the ammonia molecule (NH<sub>3</sub>) displayed. The bond length is shown as 1.02 Å and the bond angle is shown as 106.0°.</p>	BL = 1.008 Å BA = 107°  E = 0.04063 kJ/mol (after 9 steps) Molecule from "Get Mol" taken energy = 4.558 kJ/mol

2.	Water (H <sub>2</sub> O)		<p>BL = 0.957 Å<sup>o</sup></p> <p>BA = 104.5°</p> <p>E = 0.00632 kJ/mol (after 6 steps)</p> <p>Molecule from “Get Mol” taken energy = 5.669 kJ/mol</p>
3.	Aluminium Chloride (AlCl <sub>3</sub> )		<p>BL = 2.08 Å<sup>o</sup></p> <p>BA = 120°</p> <p>E = 0.01418 kJ/mol (after 22 steps)</p> <p>Molecule from “Get Mol” taken energy = 33.58 kJ/mol</p>
4.	Phosphorus Chloride (PCl <sub>3</sub> )		<p>BL = 2.07 Å<sup>o</sup></p> <p>BA = 103°</p> <p>E = 0.00090 kJ/mol (after 14 steps)</p> <p>Molecule from “Get Mol” taken energy = 6.150 kJ/mol</p>
5.	Phosphorus Pentachloride (PCl <sub>5</sub> )		<p>BL = 2.02Å<sup>o</sup> and 2.4Å<sup>o</sup></p> <p>BA = 90° and 120°</p> <p>E = 526.716492 kJ/mol (after 100 steps)</p> <p>Molecule from “Get Mol” taken energy = 548.355 kJ/mol</p>

### Methodology

Open the **Jmol app** (16.2.17-Binary). From tool bar click on “model kit” menu to draw a molecule. In the menu options you can add any element as required.

Following are the steps and ways a molecule can be drawn in “Jmol” panel:

Get Mol : In Jmol Panel go to File >> Get Mol. Readily available structure from data base is visible on the Jmol.

Draw using molecular editor: In Jmol panel go to “model kit” basic methane structure pops out. Select required element and step-wise convert it into required molecule.

(This must be separate point) Go to “Tools” >> 2D >> and draw the molecule required and use “replace 3D” option to view the 3D model on Jmol panel.

To measure bond length, keep the cursor on the molecule and right click, click on measurements. It will open up with multiple options like measure bond length in picometer, nanometer, etc. (I have used Armstrong units for bond length measurement). Similarly you can also measure bond angle between any two atoms in the molecule.

In menu bar you can click on “View” and click on “axis”. This can show orientation of a molecule in the chosen coordinate plane.

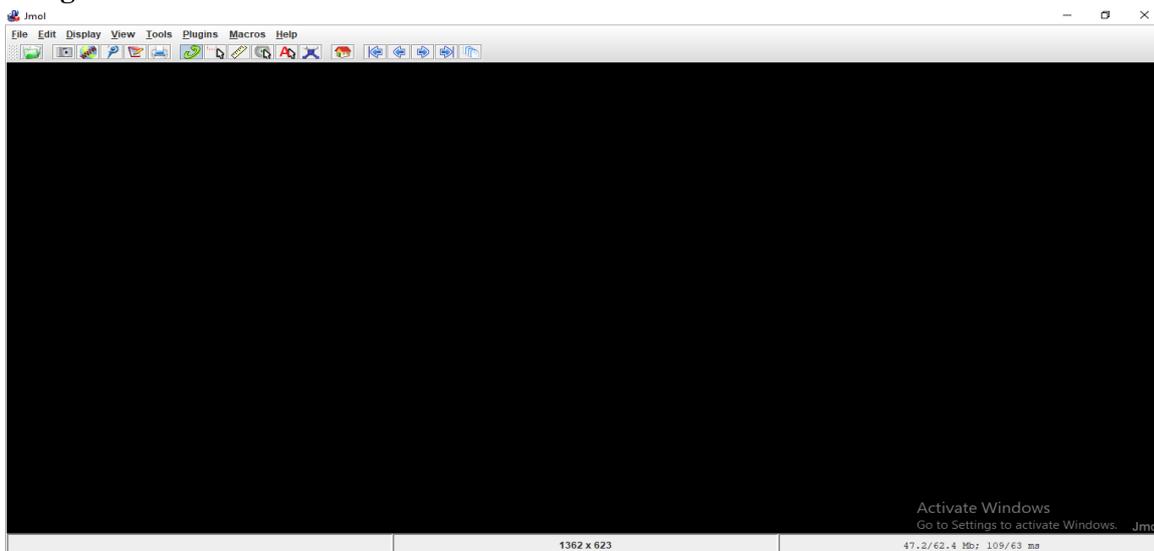
Using rotate tool molecule can be rotated to view 3D model from various angles: front, back, top and bottom view.

Molecule can be loaded on the Jmol panel from “Get Mol” option. The structure of molecules can be retrieved from the database by typing the name/CAS/SMILES/InChi key.

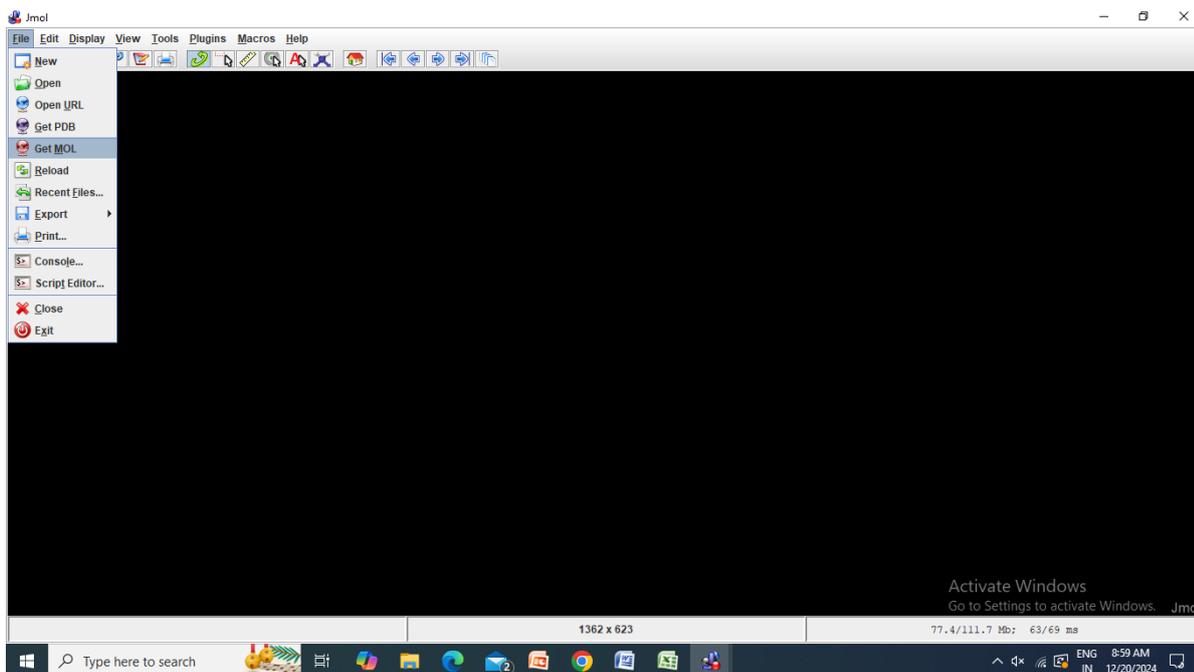
Using “model kit” menu minimize the energy of a molecule. Using “minimize” option.

The click on “File >> Console” option to view the energy of the molecule.

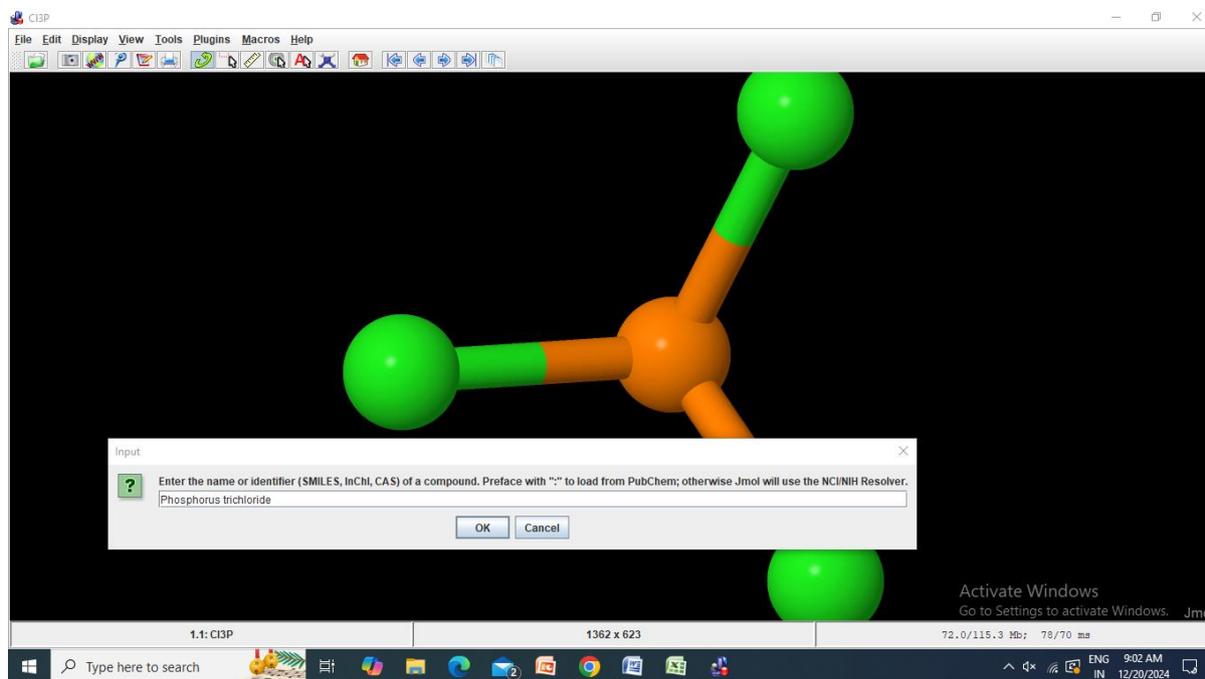
**Image 1:** Jmol Interface



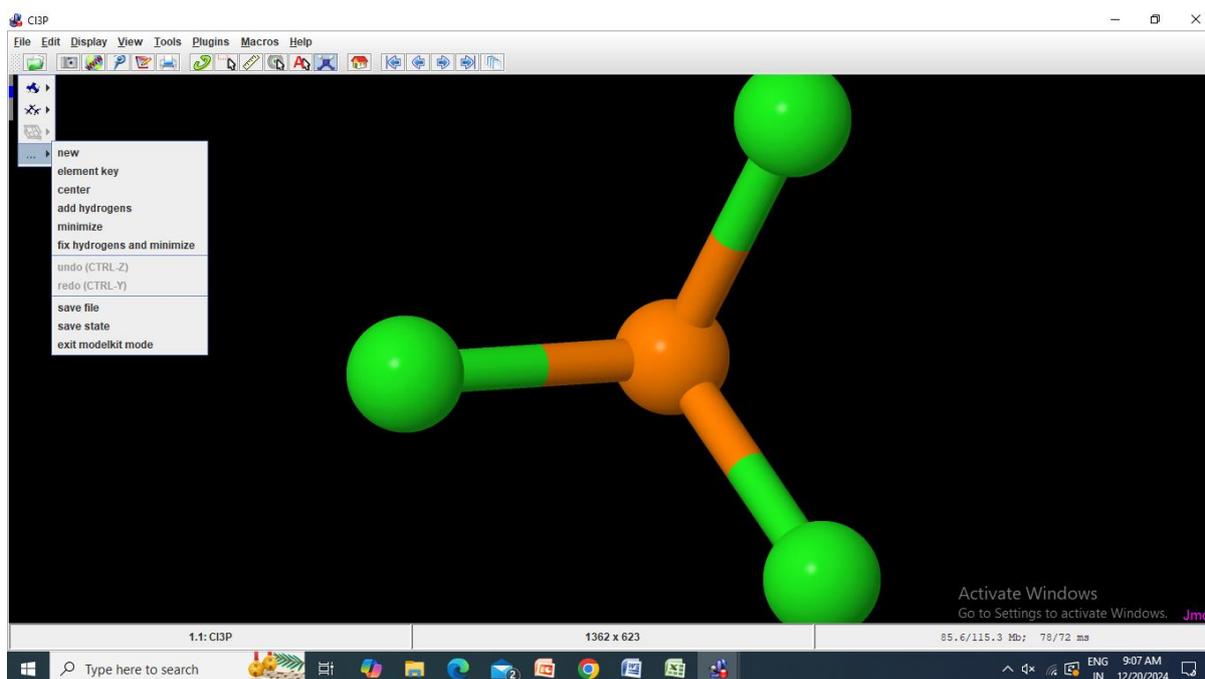
**Image 2:** Get a molecule from “Get Mol” date base of molecules.



**Image3:** Click on “Get Mol” text box open up. Required molecule is obtained by typing or pasting the name of a molecule, CAS number or Smiles of a molecule.

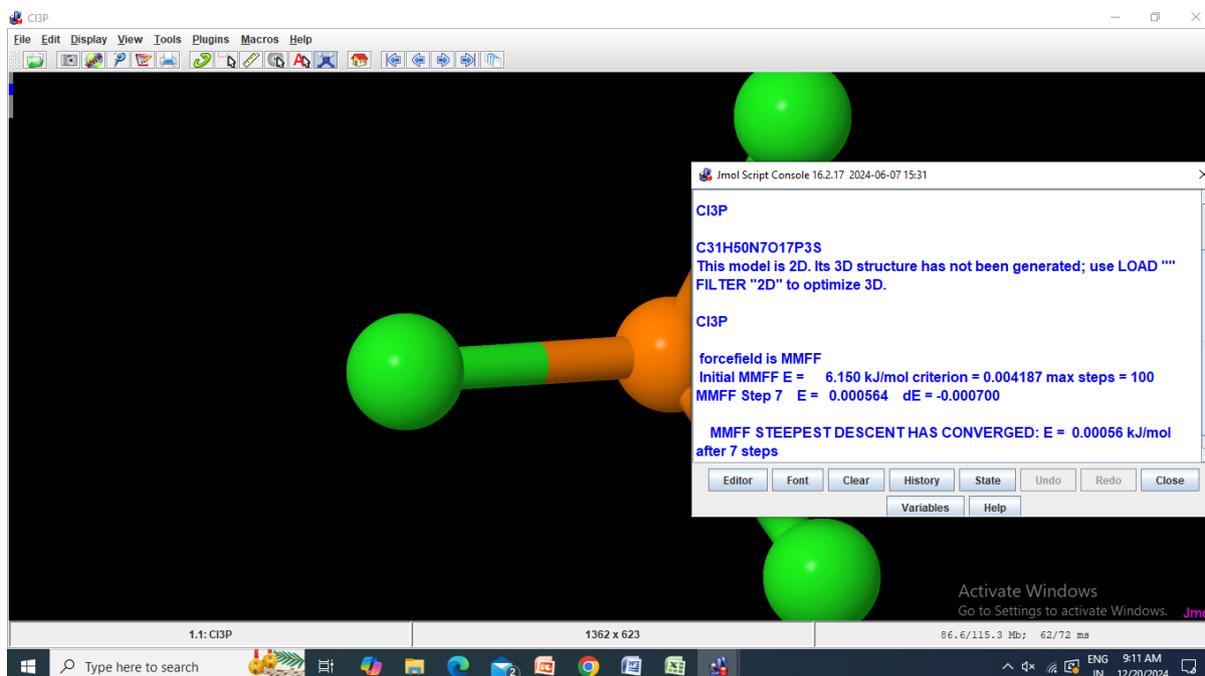


**Image 4:** To determine the energy of a molecule: Click on model kit menu minimise.



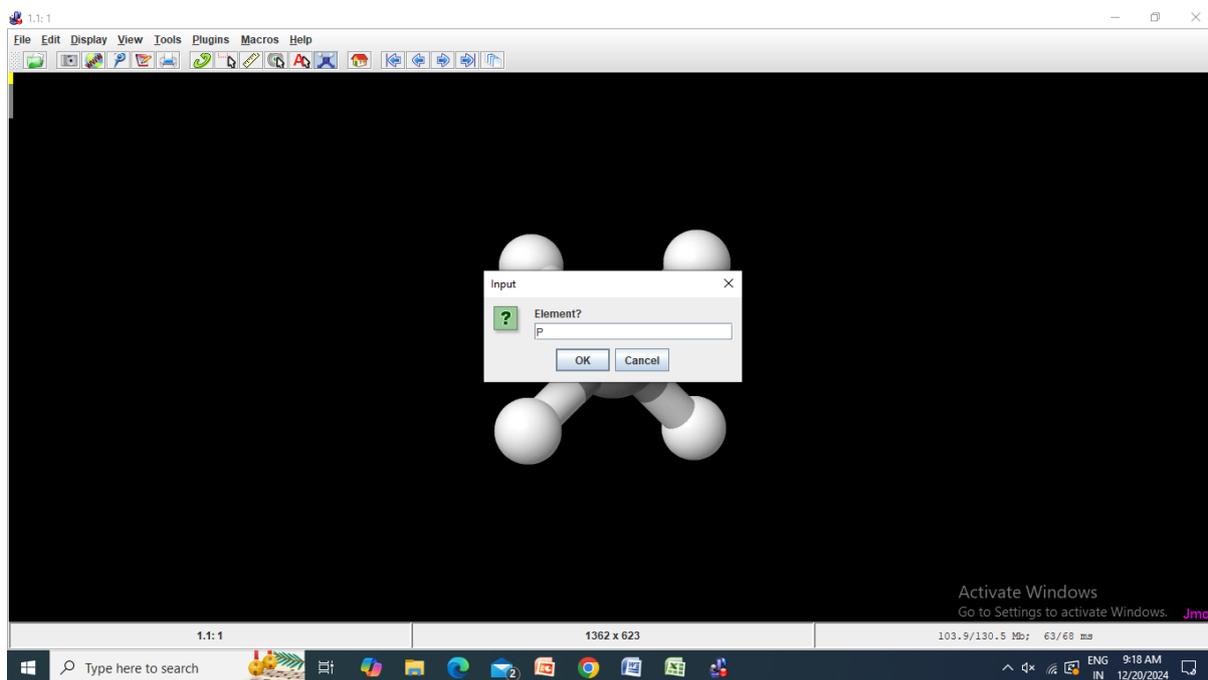
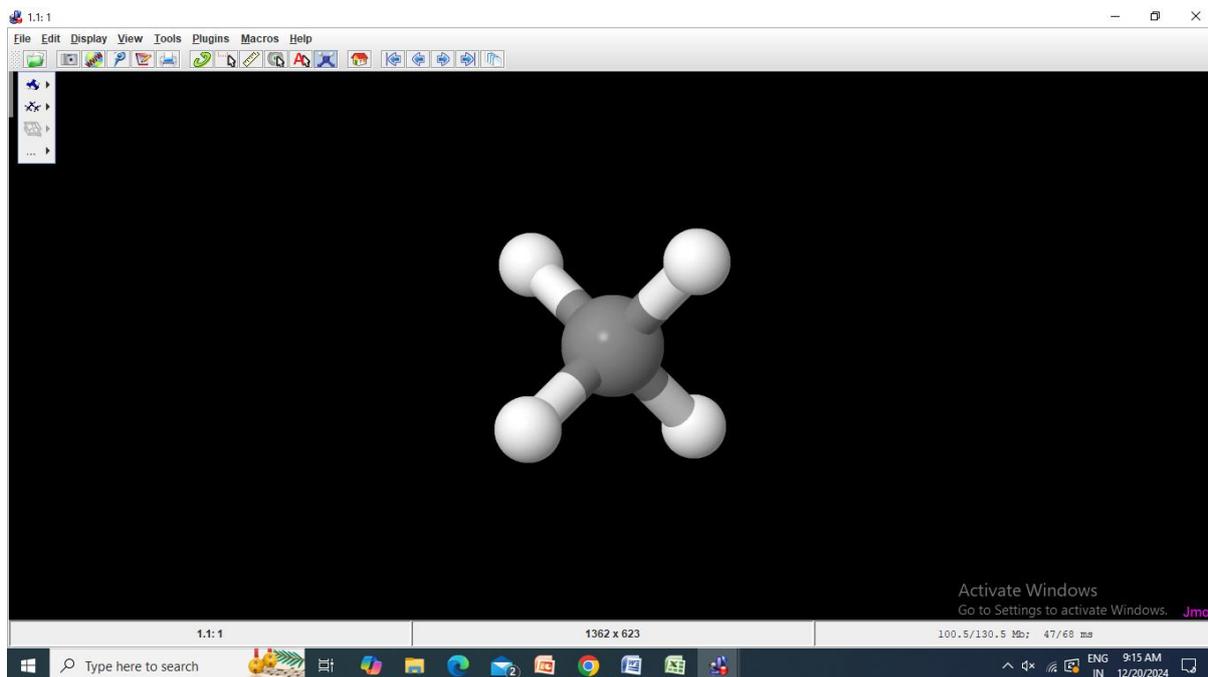
**Note:**

When we take a molecule from “Get Mol” we take initial energy of the molecule (For example  $\text{PCl}_5$  = 6.150 kJ/mol) whereas when we draw a molecule we take final energy with the number of steps involved in drawing the molecule. (Shown below)

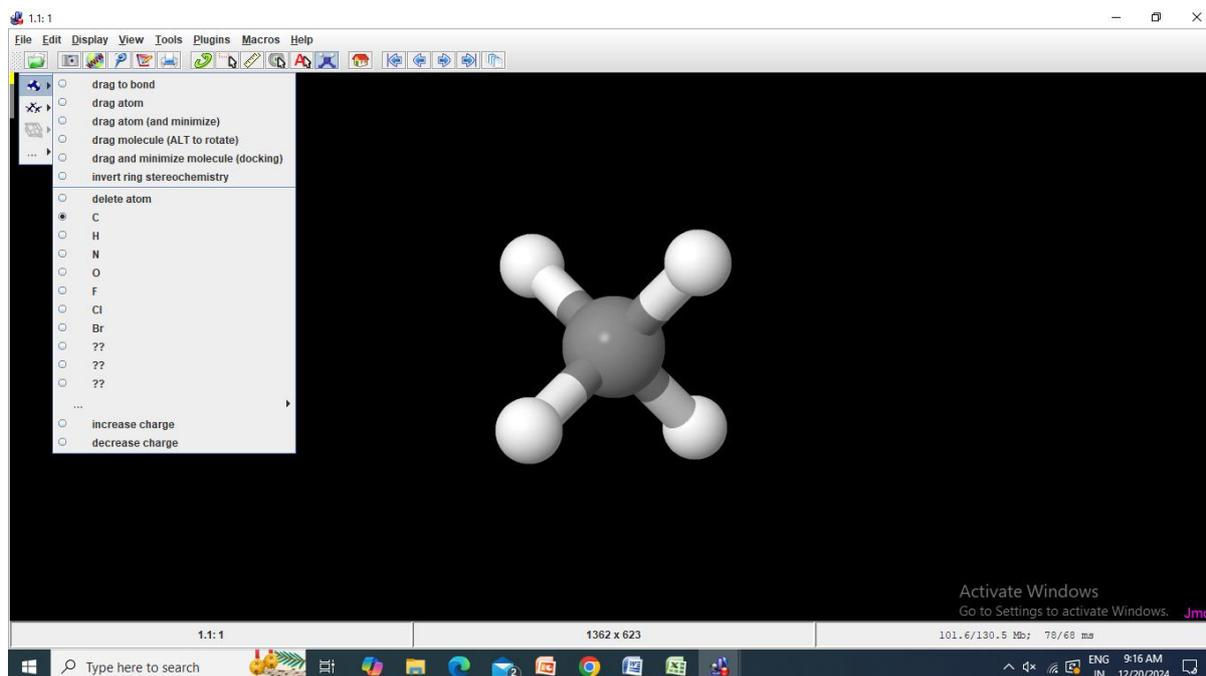


Creating the 3D model, using molecular editor

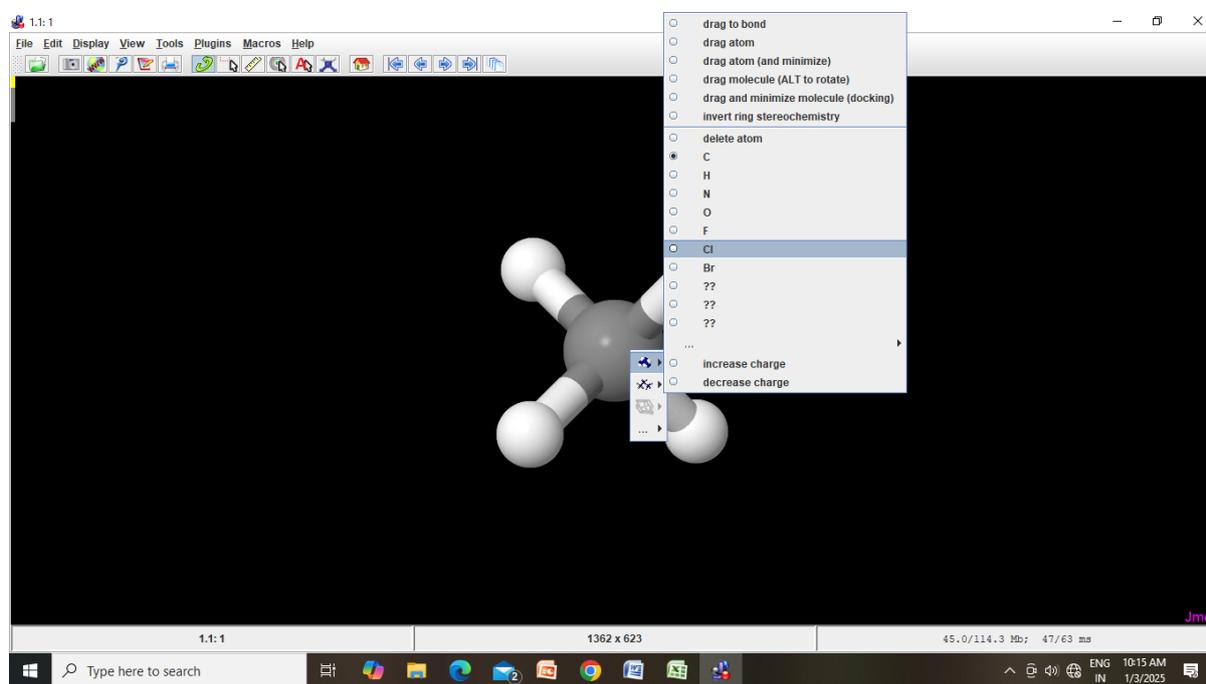
**Image 5:** Click on “model kit tool” methane molecule is displayed.



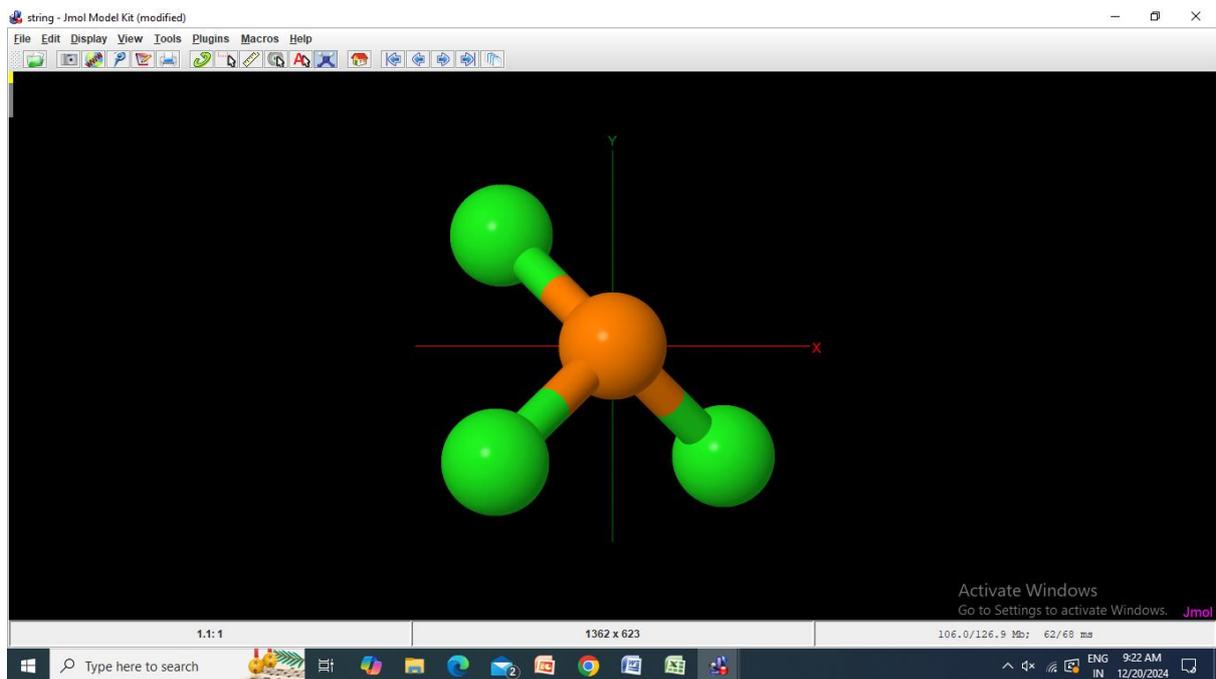
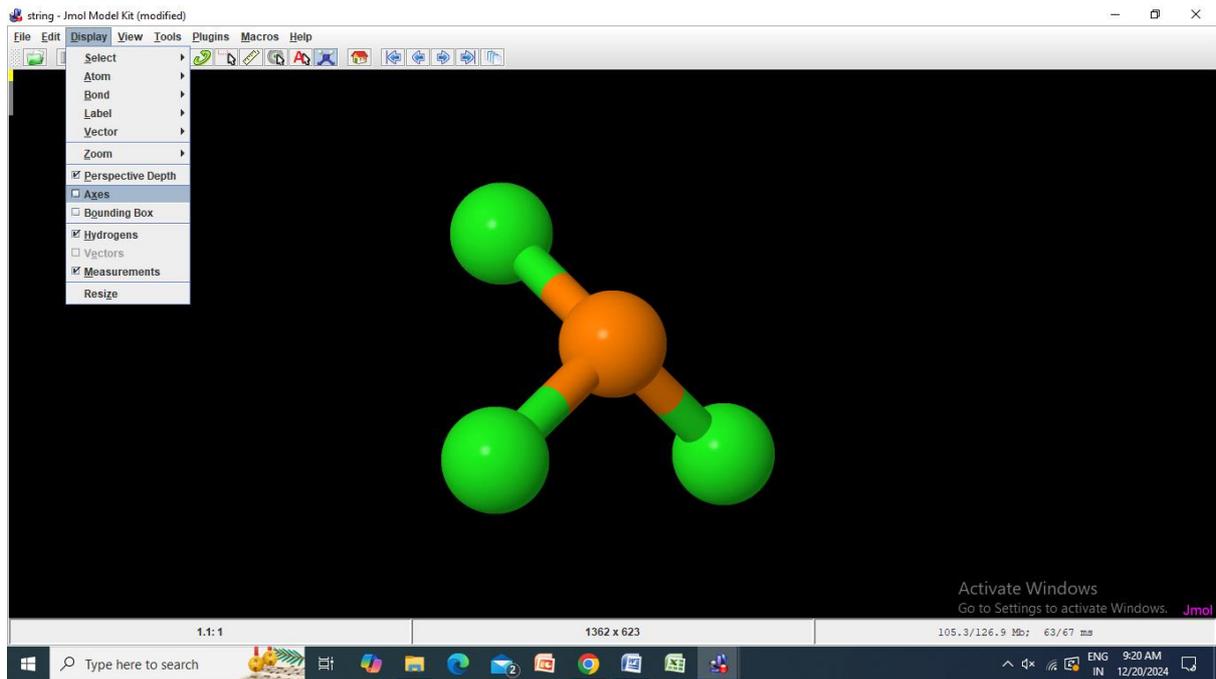
**Image 6:** Click on model kit common elements are shown and “?” is to add the element of choice. For example “P” and “Cl” to make Phosphorus trichloride (PCl<sub>3</sub>).



**Image 7:** Change Atom to make the required molecule



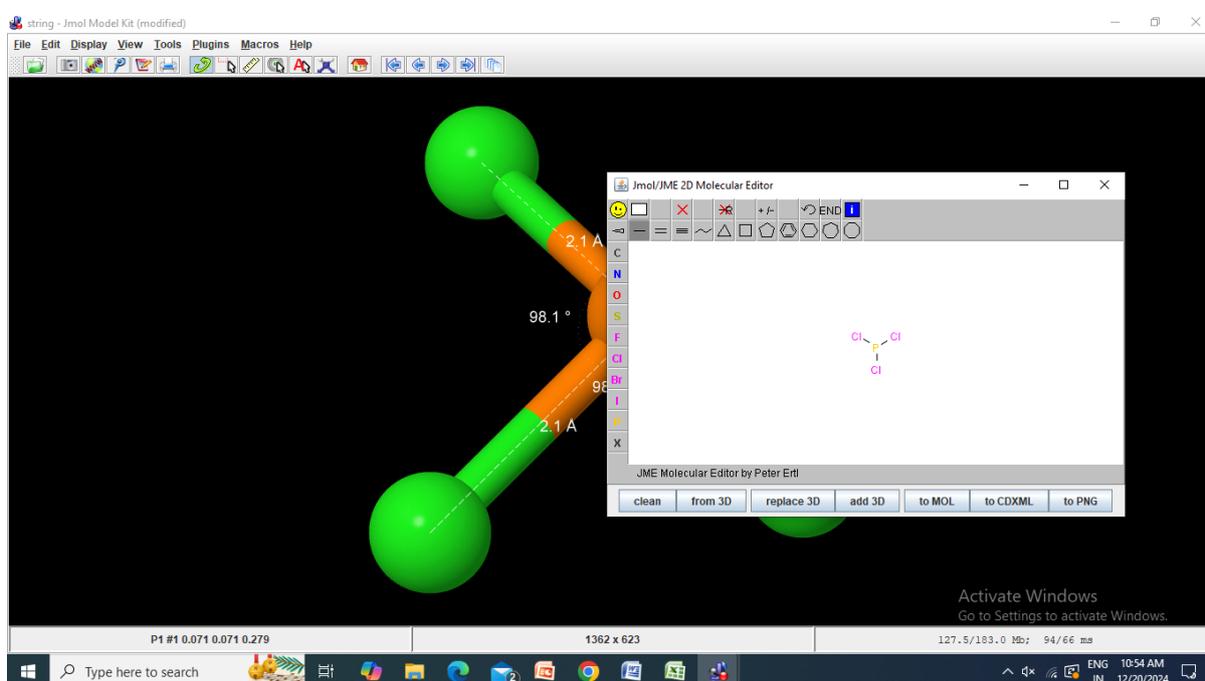
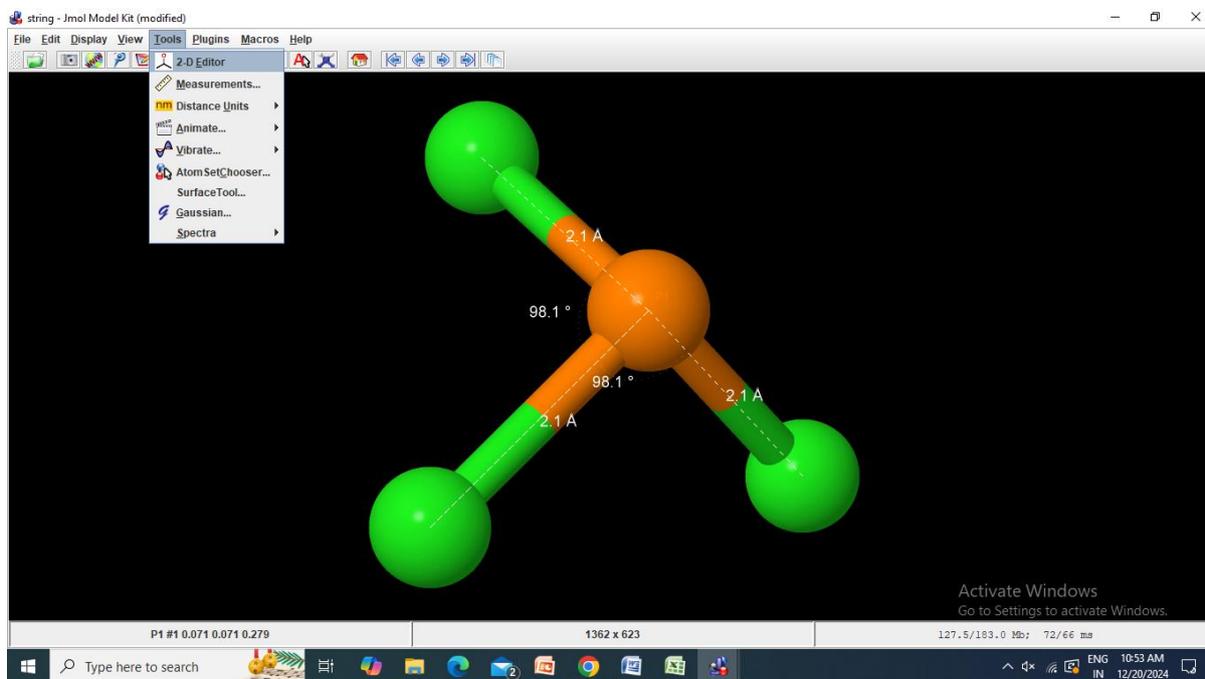
**Image 8:** To show axis click on Display >> Axes



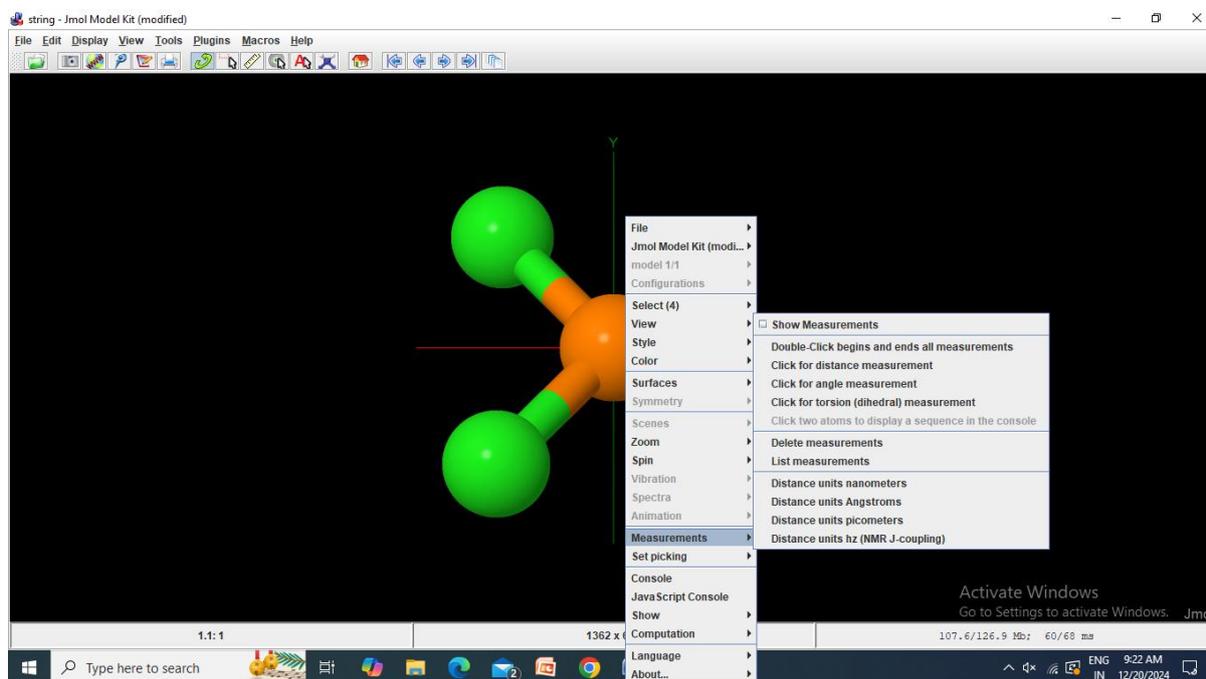
**Image 8:** 2-D Editor option to draw molecule on Jmol panel:

Select 2-D Editor option from Tools menu.. A separate window Jmol/JME 2D molecular editor window opens.

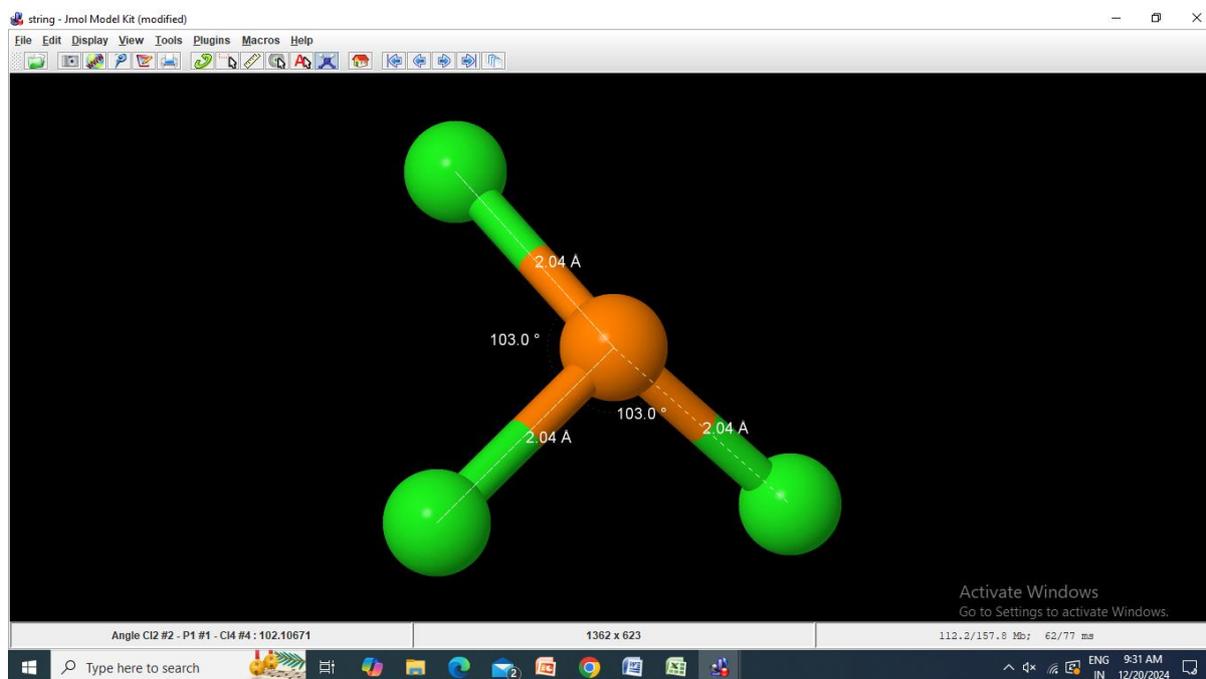
Draw the 2D drawing using the features in the window. Click on “replace 3D” to view model on Jmol panel.



**Image 9:** To measure bond length and bond angle click on ruler image in menu bar >> Double click on an atom and move the cursor to next atom, the bond length is visible for the two selected atoms. Similarly as atoms are selected bond angle value is also measured. Below image shows the menu items for measurements in different units.

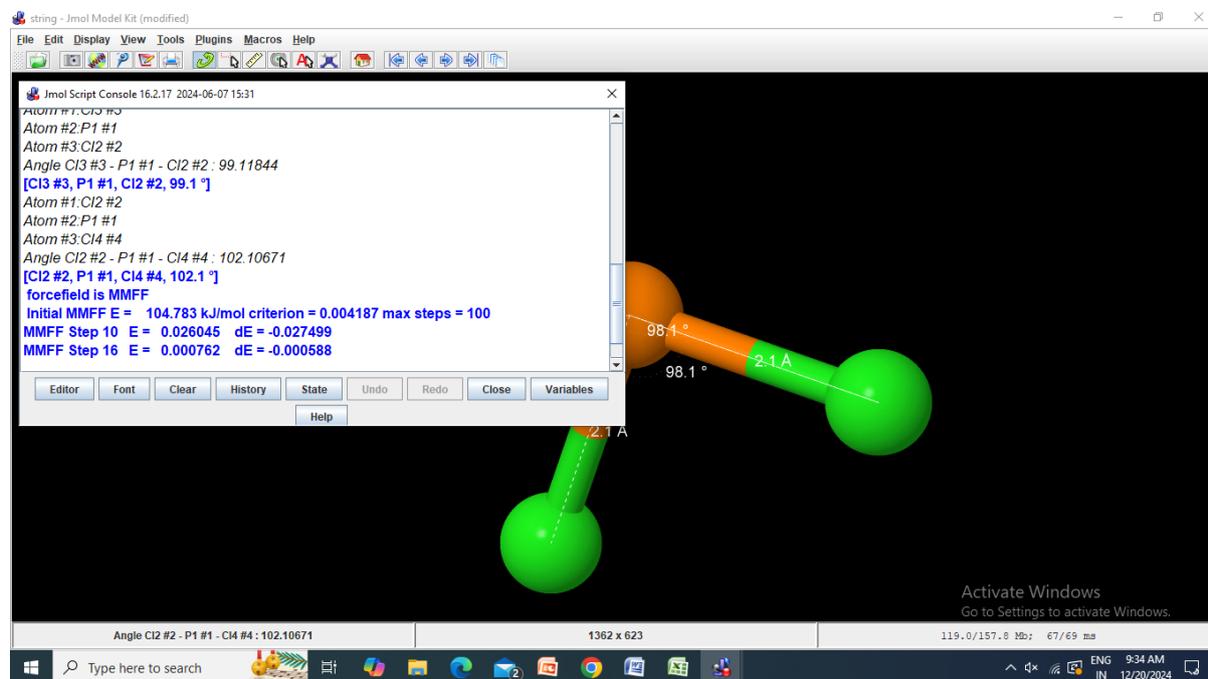


**Image 10:** Measurements for  $\text{PCl}_5$  are visible for the molecule



After drawing the molecule minimise using minimize option in the model kit menu. Open the console using File menu to see the energy of the molecule.

**Image 11:** In this Energy minimization is a multiple steps process we take the final step energy. It also shows stepwise energy change of the molecule.



## Results and Discussions:

In this project we have used Jmol 3D visualization software to draw the molecule and to determine bond length and bond angle of a molecule. We have also compared the stability of molecules by determining the energies of the molecules. The molecules with high energy values are less stable compared to the molecules with low energy.

When we compare the energy of  $\text{PCl}_3$  6.150 kJ/mol and  $\text{PCl}_5$ , 548.355 kJ/mol (later shows higher energy compare to  $\text{PCl}_3$  and therefore  $\text{PCl}_5$  is more reactive compare to  $\text{PCl}_3$ ).

Reactivities of  $\text{AlCl}_3$  (33.58 kJ/mol),  $\text{PCl}_3$  (6.150 kJ/mol),  $\text{PCl}_5$  (548.355 kJ/mol) are more when compared to water (5.669 kJ/mol) or ammonia (4.558 kJ/mol) as indicated by their energy after minimization.

## Conclusion:

Jmol app is user friendly. It can help teachers to explain the concepts using 3D models. Students can also try 3D modelling for comparison of parameters such as bond angle, bond length, energies of different molecules. Its “minimise” feature helps to stabilise the molecule in most stable orientation (to reduce or minimise lone pair-lone pair, bond pair bond pair and bond pair-lone pair interactions). The energy of a stable molecule is calculated using the inbuilt Force Field computational method. Calculations can be obtained by opening the “Console” using File menu. The energy in kJ/mol for each molecule can be compared to analyze their reactivity.

Reference:

[https://chem.libretexts.org/Bookshelves/Introductory\\_Chemistry/Introductory\\_Chemistry\\_\(CK-](https://chem.libretexts.org/Bookshelves/Introductory_Chemistry/Introductory_Chemistry_(CK-12)/08%3A_Ionic_and_Metallic_Bonding/8.02%3A_Octet_Rule#:~:text=The%20octet%20rule%20states%20that,only%20has%20two%20valence%20electrons.)

[12\)/08%3A\\_Ionic\\_and\\_Metallic\\_Bonding/8.02%3A\\_Octet\\_Rule#:~:text=The%20octet%20rule%20states%20that,only%20has%20two%20valence%20electrons.](https://chem.libretexts.org/Bookshelves/Introductory_Chemistry/Introductory_Chemistry_(CK-12)/08%3A_Ionic_and_Metallic_Bonding/8.02%3A_Octet_Rule#:~:text=The%20octet%20rule%20states%20that,only%20has%20two%20valence%20electrons.)

NCERT class 11 Chemistry Part 1 textbook.

Shiver Atkins, Inorganic Atkins, 5th Edition Oxford India Edition

[https://chem.libretexts.org/Bookshelves/Inorganic\\_Chemistry/Supplemental\\_Modules\\_and\\_Websites\\_\(Inorganic\\_Chemistry\)/Descriptive\\_Chemistry/Elements\\_Organized\\_by\\_Period/Period\\_3\\_Elements/Chlorides\\_of\\_Period\\_3\\_Elements](https://chem.libretexts.org/Bookshelves/Inorganic_Chemistry/Supplemental_Modules_and_Websites_(Inorganic_Chemistry)/Descriptive_Chemistry/Elements_Organized_by_Period/Period_3_Elements/Chlorides_of_Period_3_Elements)