

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 PCl_3 , PCl_5 , 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:

¹The 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.

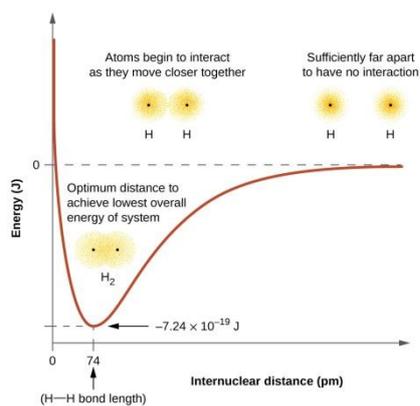
Valence bond theory:

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:

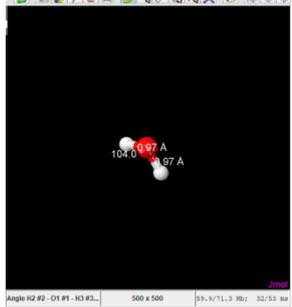
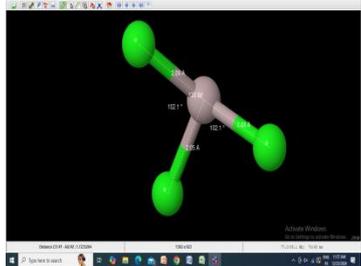
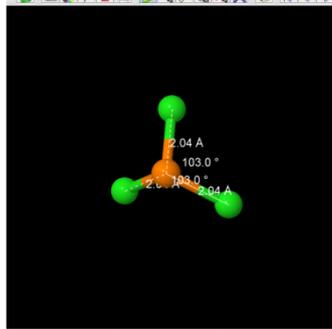
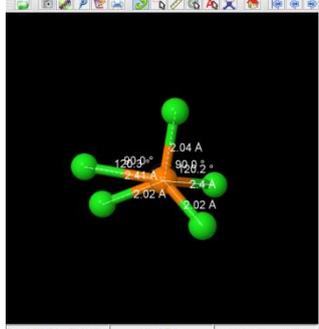
Valence Shell Electron Pair Repulsion Theory (VSEPR) explains about geometry of molecules. It explains the three dimensional orientation of molecules in XYZ plane. This theory considers lone pair and bond pair of electrons in a molecule for predicting the geometry and orientation of a molecule.

Problem:

To measure bond length and bond angle of the following molecules using Jmol Application. Phosphorus trichloride (PCl₃), Phosphorus pentachloride (PCl₅), Aluminium chloride (AlCl₃), Water (H₂O) and Ammonia (NH₃)
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 Geometry
1.	Ammonia (NH ₃)	<p>The screenshot shows the Jmol application window with a ball-and-stick model of ammonia (NH₃). The bond length is displayed as 1.02 Å and the bond angle is 106.0°. The status bar at the bottom shows 'Angle H2 #2 - N1 #1 - H4 #4...' and '500 x 500'.</p>	BL = 1.008 Å ^o BA = 107 ^o E = 0.04063 kJ/mol (after 9 steps) Molecule from "Get Mol" taken energy = 4.558 kJ/mol Trigonal Pyramidal

2.	Water (H ₂ O)		<p>BL = 0.957 Å^o</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> <p>Bent, distorted tetrahedral</p>
3.	Aluminium Chloride (AlCl ₃)		<p>BL = 2.08 Å^o</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> <p>Trigonal Planar</p>
4.	Phosphorus Chloride (PCl ₃)		<p>BL = 2.07 Å^o</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> <p>Trigonal pyramidal</p>
5.	Phosphorus Pentachloride (PCl ₅)		<p>BL = 2.02Å^o and 2.4Å^o</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> <p>Trigonal bipyramidal</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 draw in “**Jmol**” panel:

Get Mol : In Jmol Pannel 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

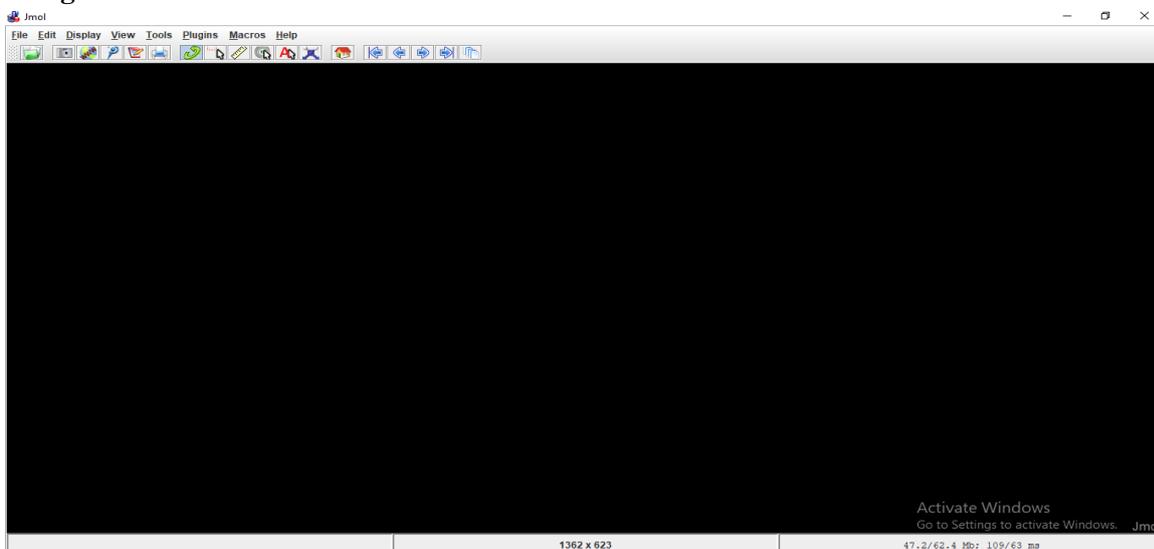


Image 2: Get a molecule from “Get Mol” date base of molecules.

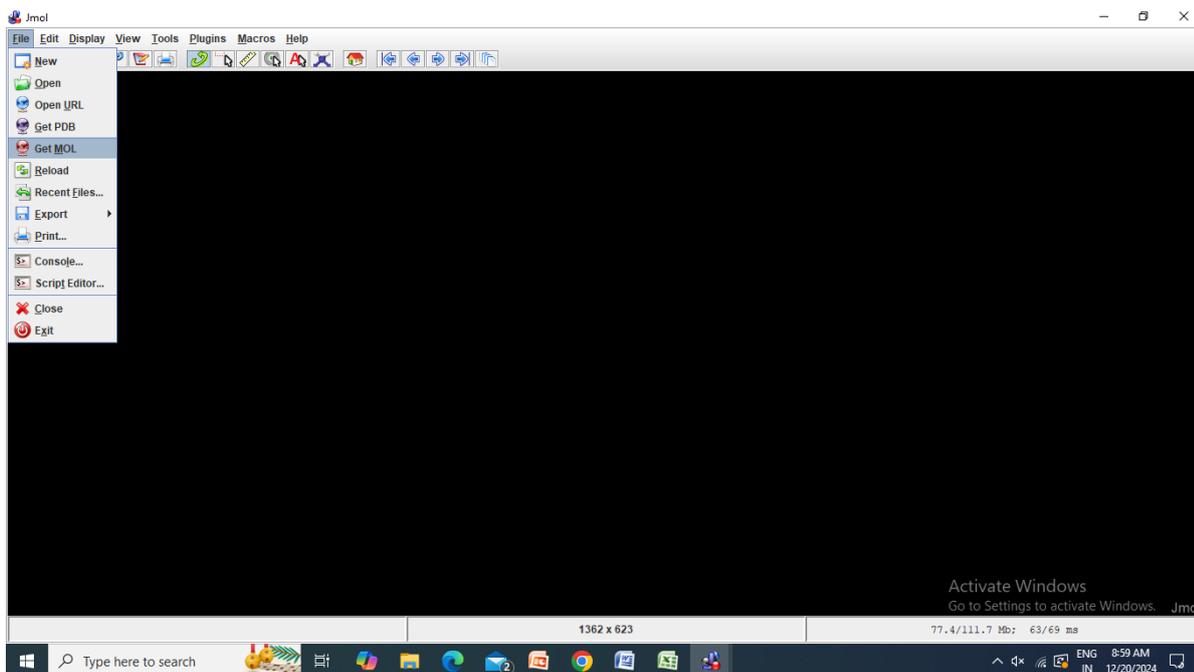


Image3: Click on “Get Mol” text box open up. Required molecule is obtained by typing or pasting the name of a molecule, CAS number or Smiles of a molecule.

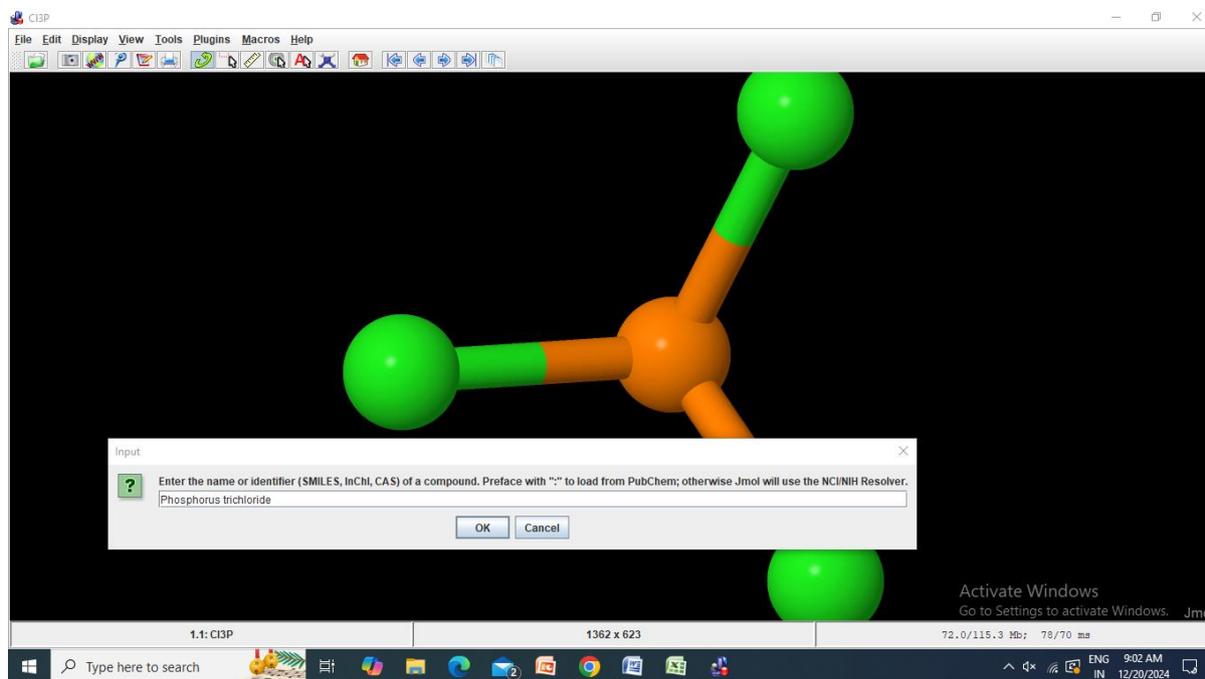
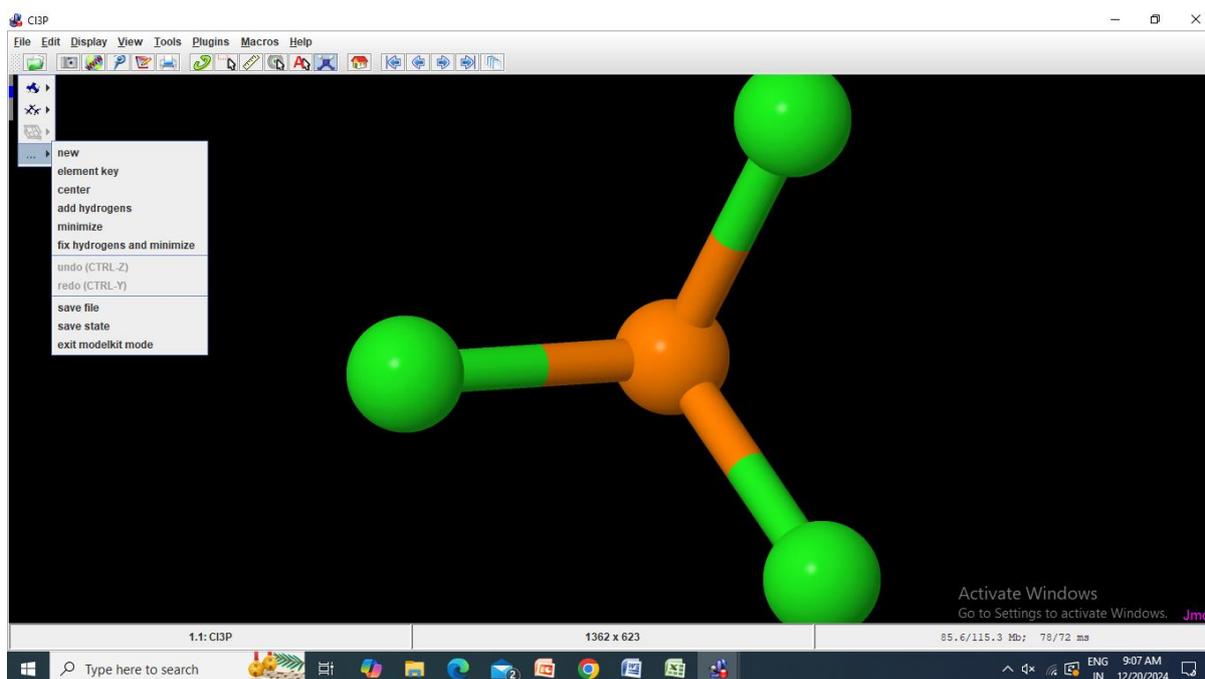
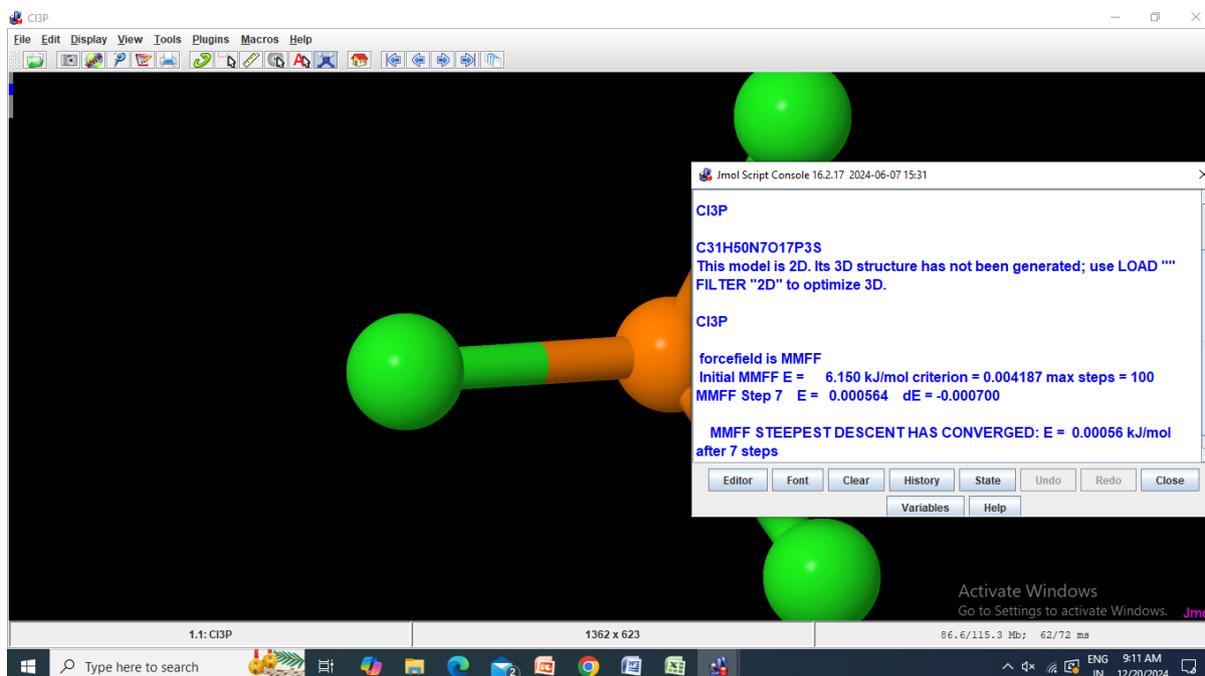


Image 4: To determine the energy of a molecule: Click on model kit menu minimise.



Note:

When we take a molecule from “Get Mol” we take initial energy of the molecule (For example 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.

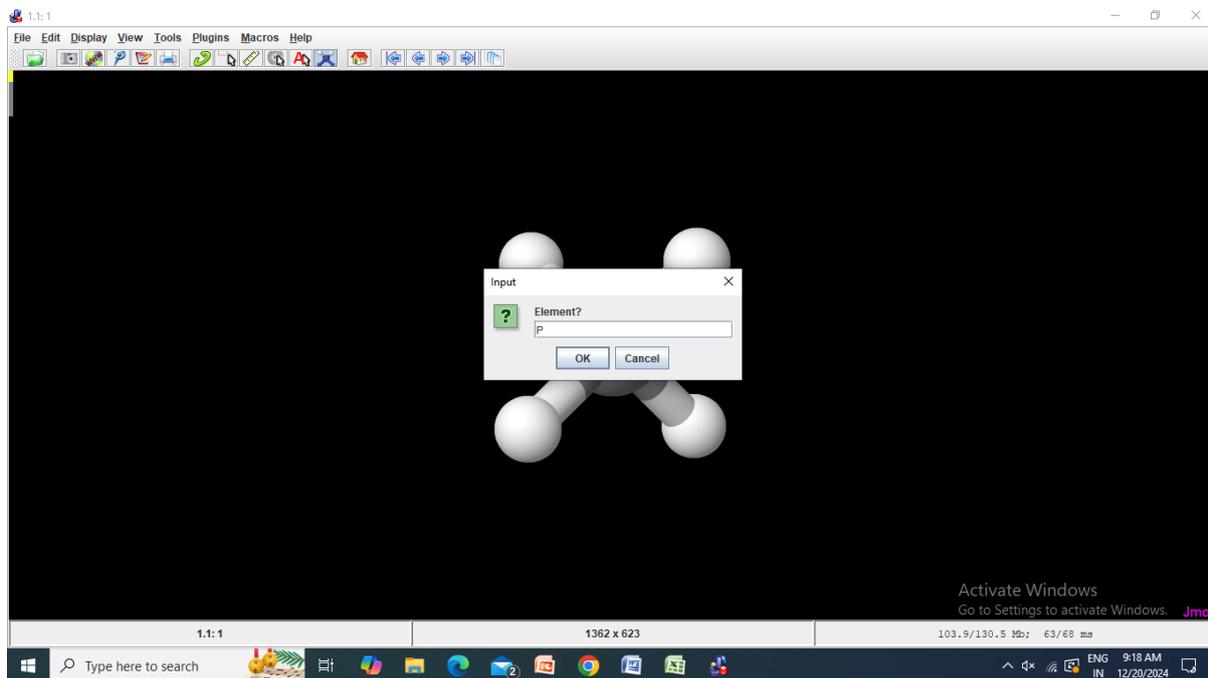
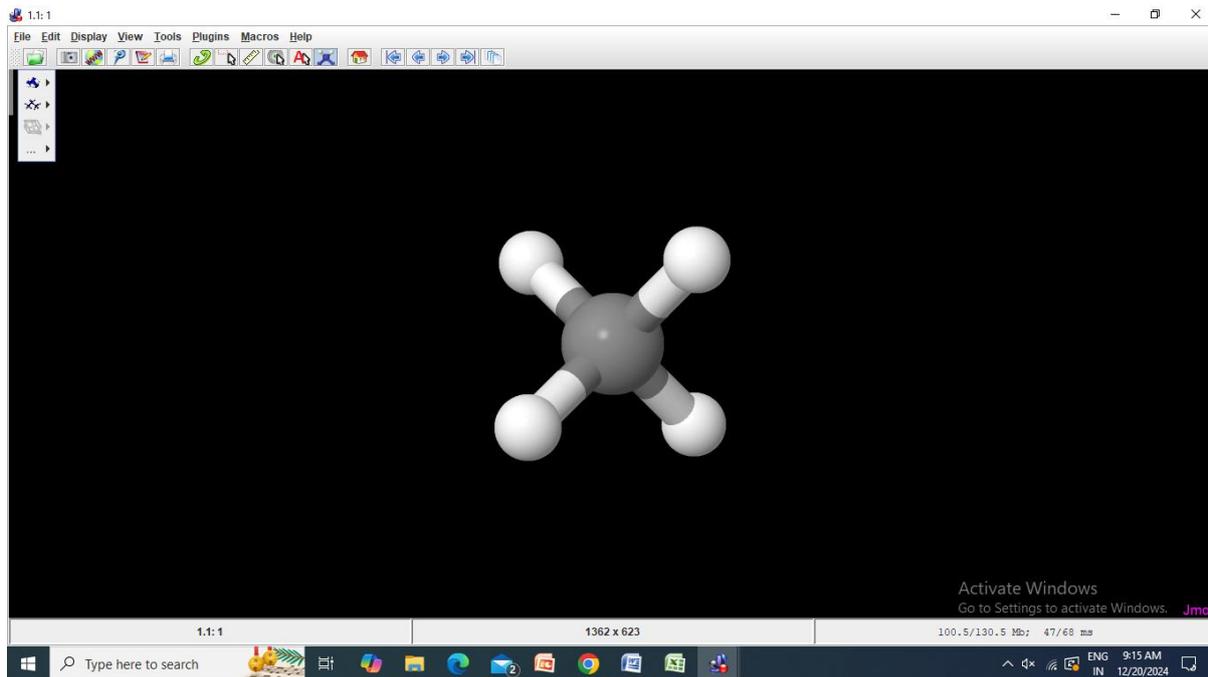


Image 6: Click on model kit common elements are shown and “?” is to add the element of choice. For example “P” and “Cl” to make Phosphorus trichloride (PCl_3).

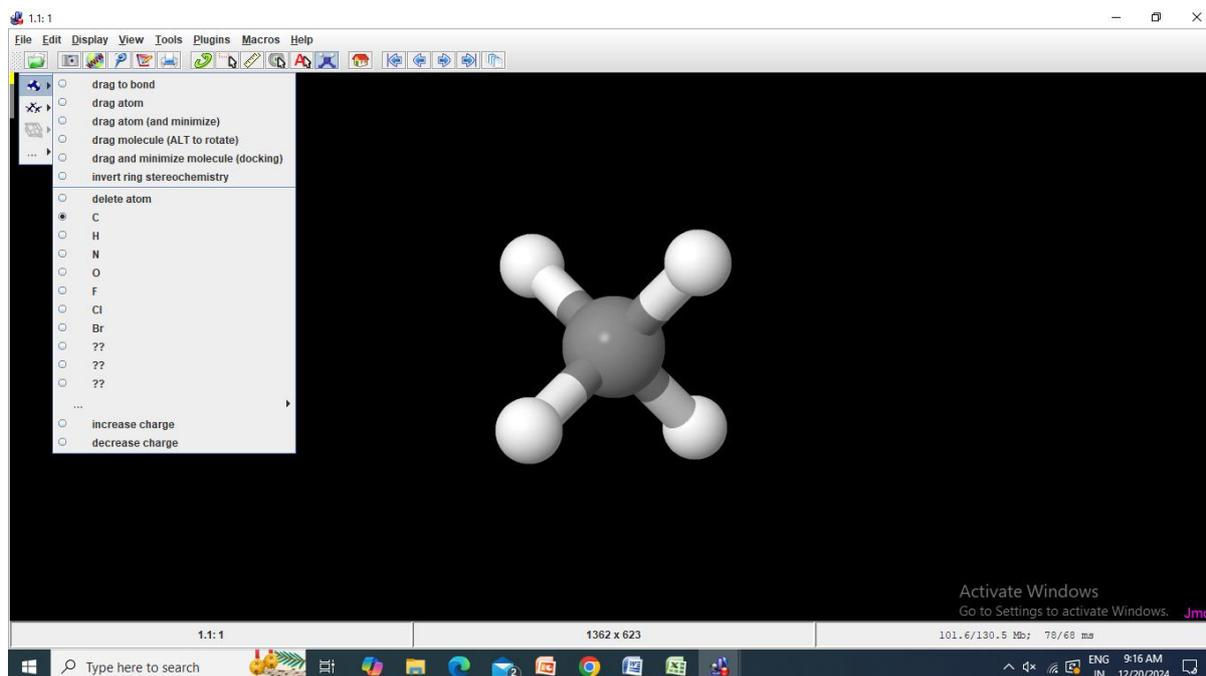


Image 7: Change Atom to make the required molecule

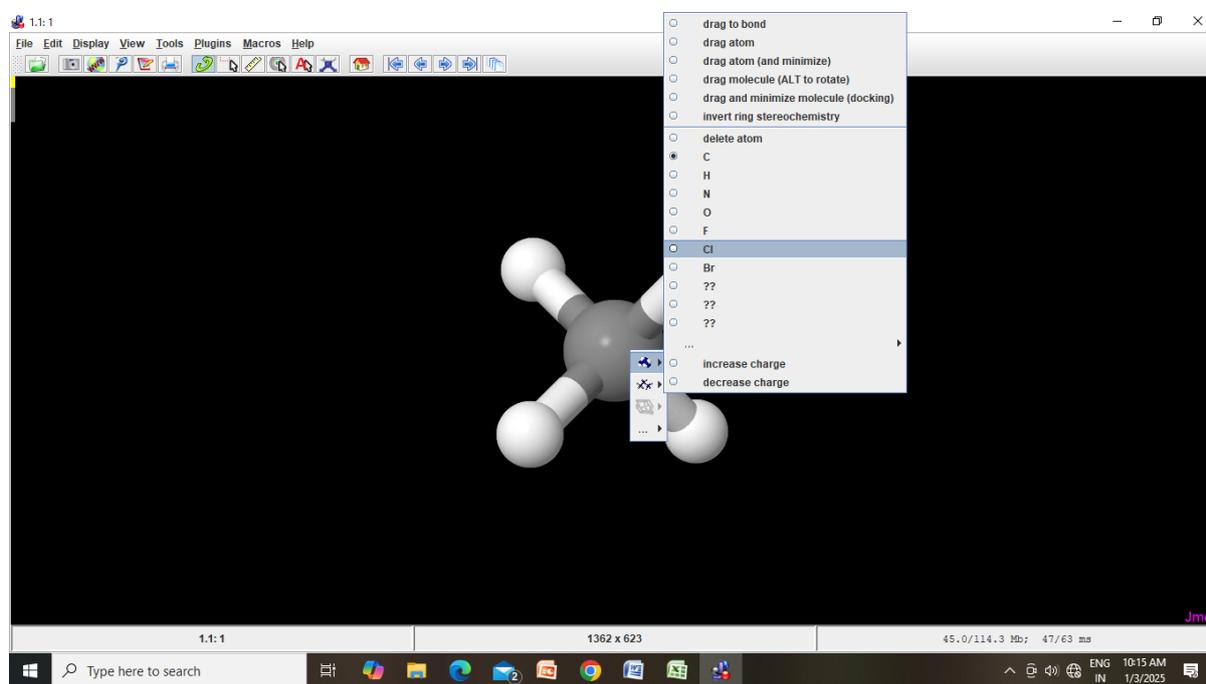


Image 8: To show axis click on Display >> Axes

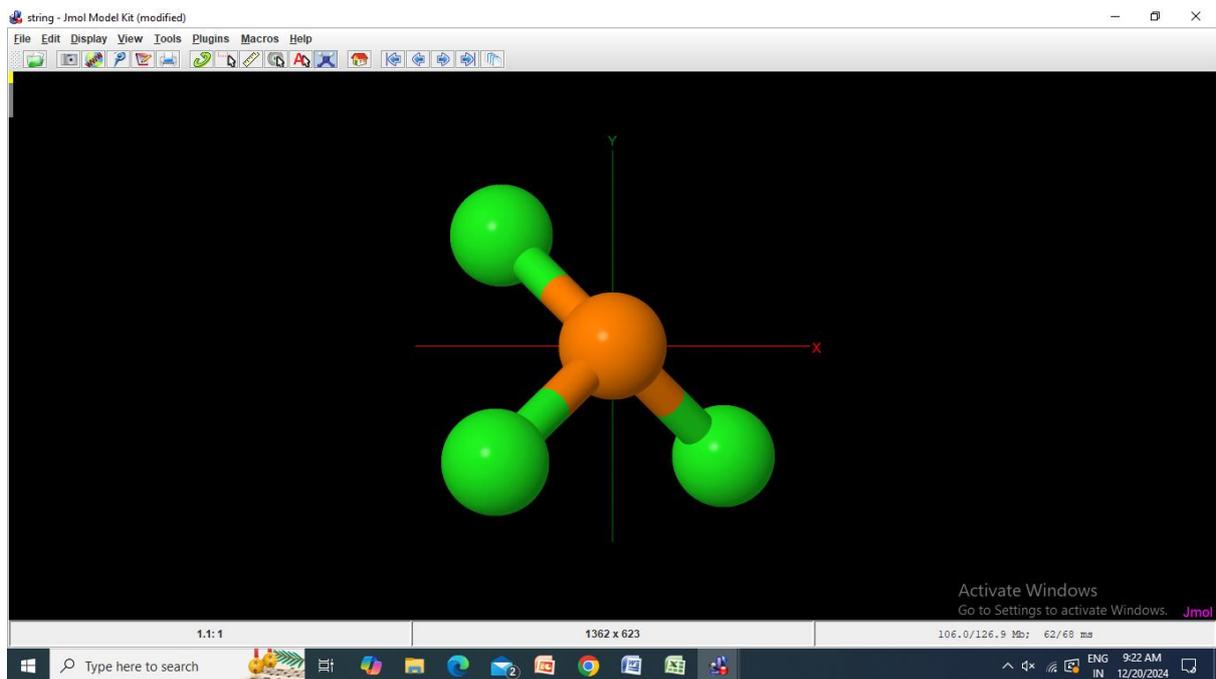
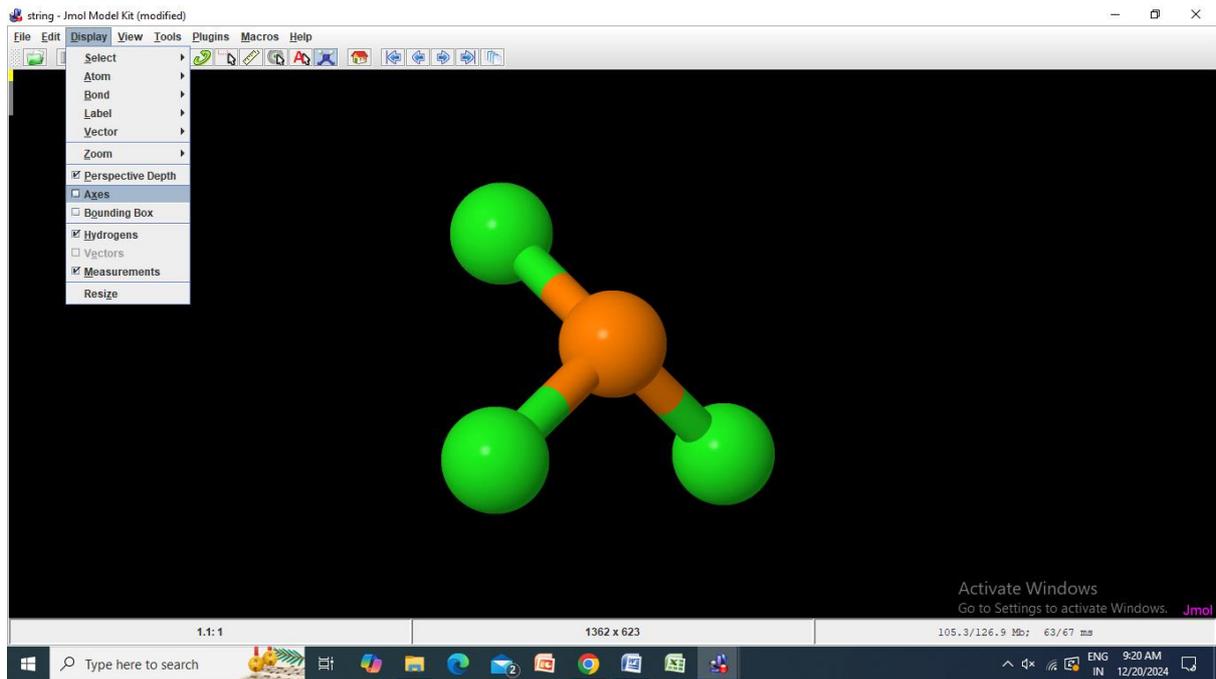


Image 8: 2-D Editor option to draw molecule on Jmol panel:

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.

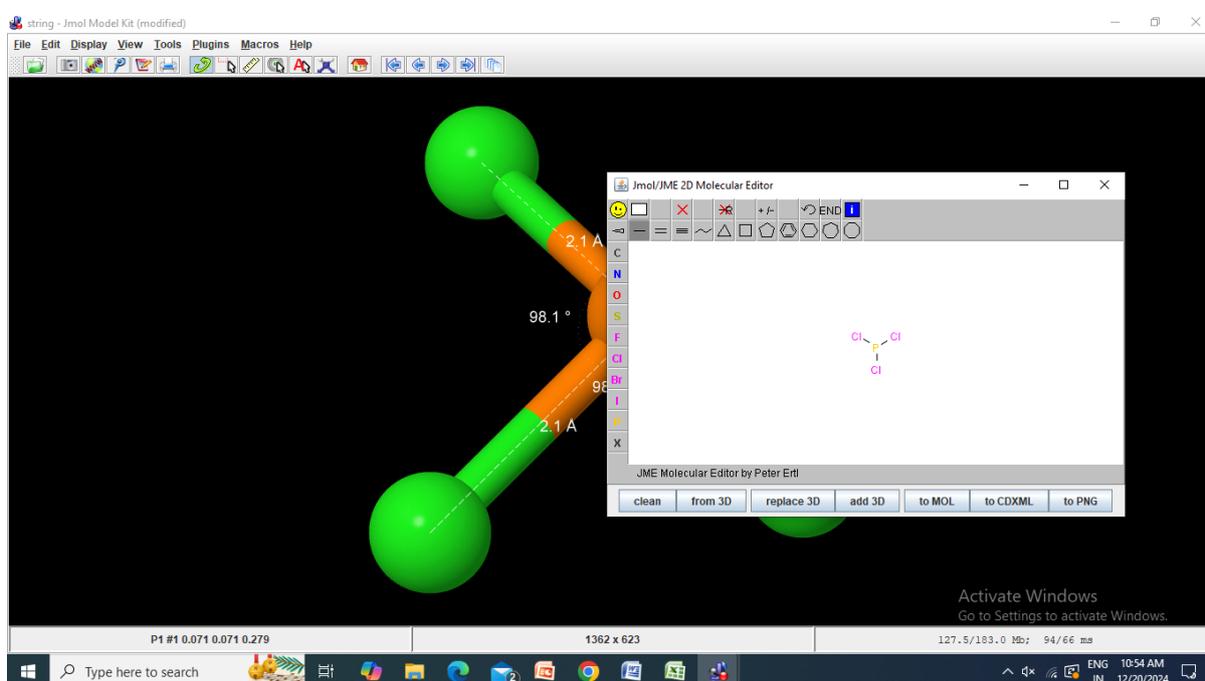
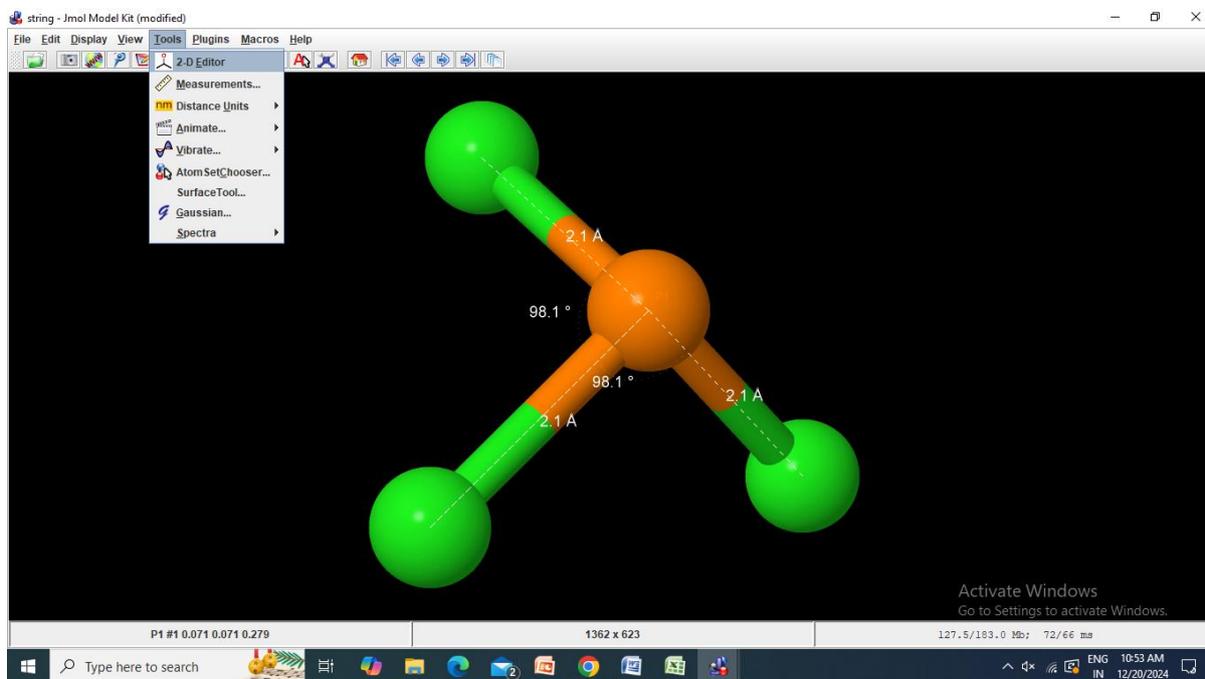


Image 9: To measure bond length and bond angle click on ruler image in menu bar >> Double click on an atom and move the cursor to next atom, the bond length is visible for the two selected atoms. Similarly as atoms are selected bond angle value is also measured. Below image shows the menu items for measurements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

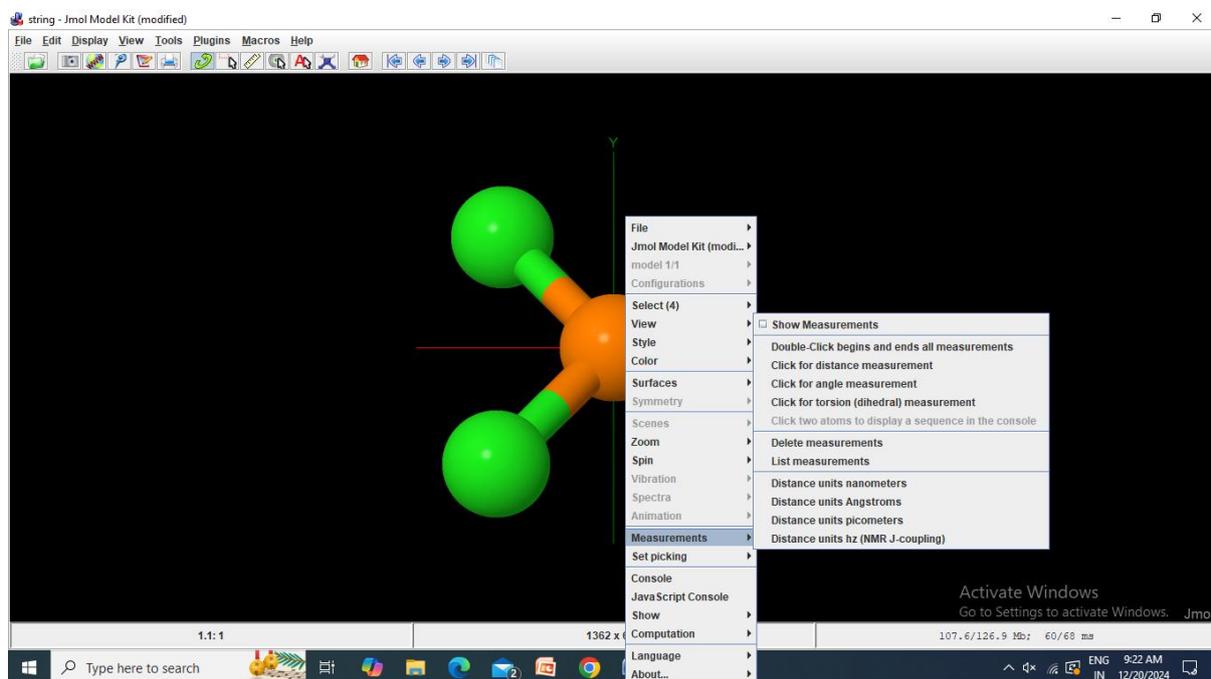
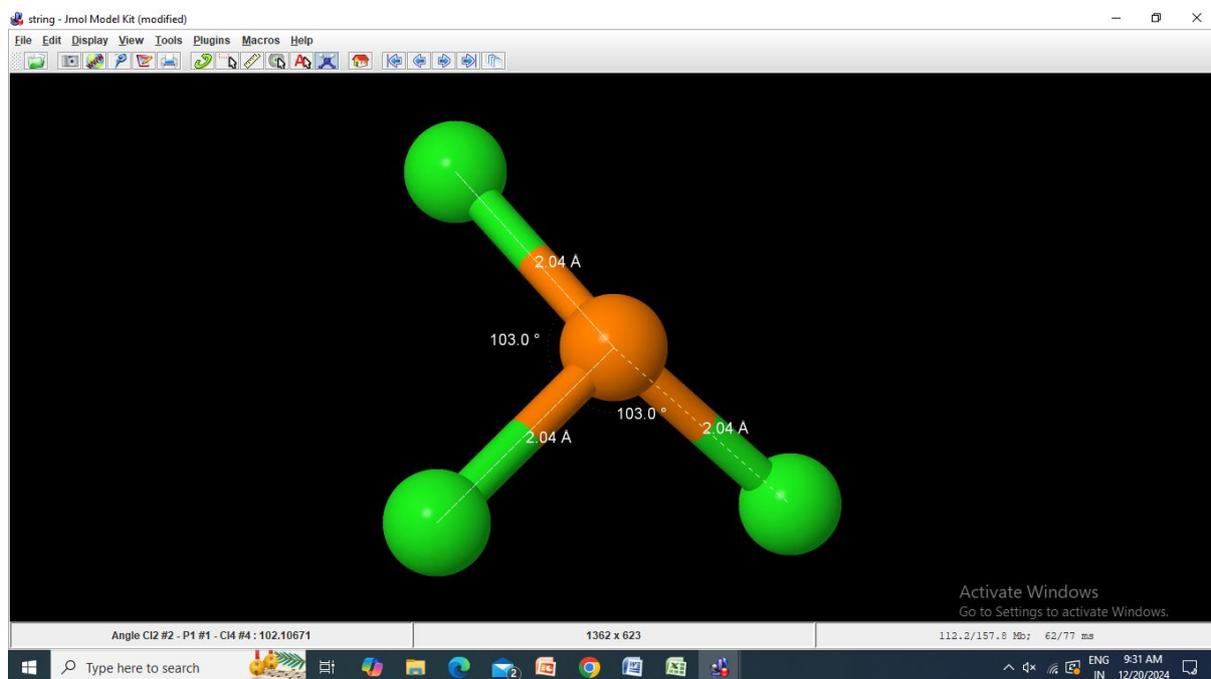
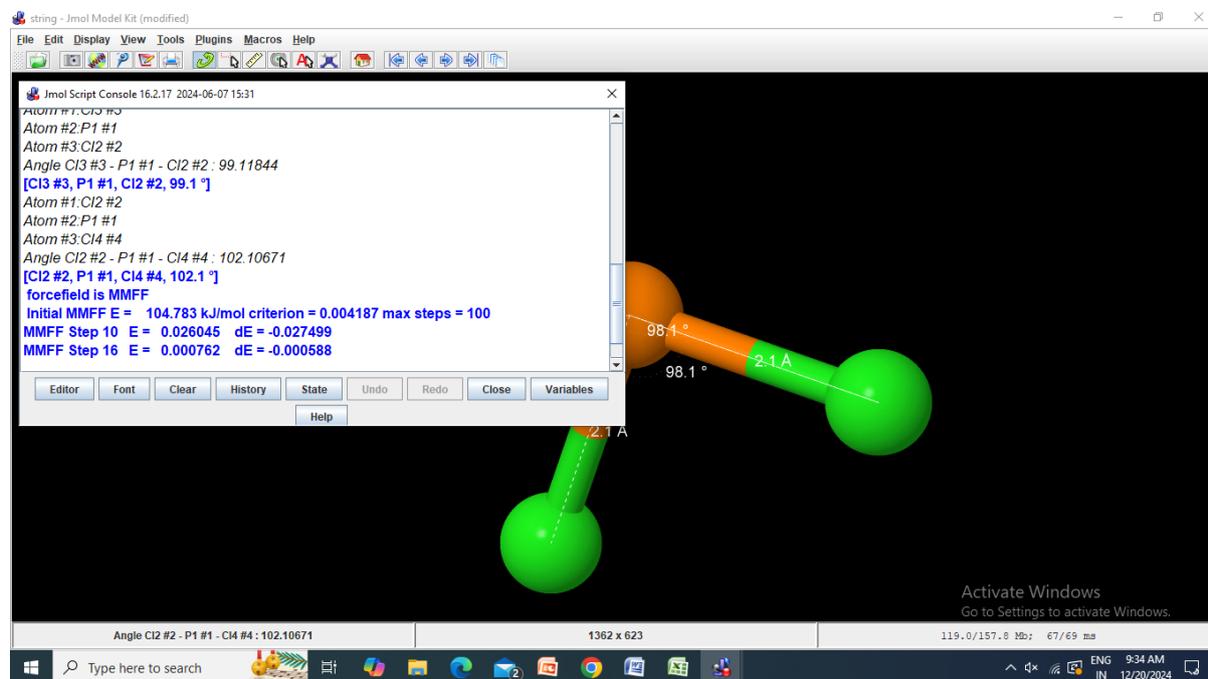


Image 10: Measurements for PCl_5 are visible for the molecule



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 PCl_3 6.150 kJ/mol and PCl_5 , 548.355 kJ/mol (later shows higher energy compare to PCl_3 and therefore PCl_5 is more reactive compare to PCl_3).

Reactivities of AlCl_3 (33.58 kJ/mol), PCl_3 (6.150 kJ/mol), 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.

Ammonia (NH_3) is a trigonal pyramidal with bond angle 107° . Nitrogen contains a lone pair of electron. There is lone pair and bond pair repulsion which reduces the bond angle of ammonia from 109° to 107° . The geometry of a molecule changes from tetrahedral to trigonal pyramidal shape. In water, oxygen is a central atom bonded with two hydrogen atoms; the expected geometry is tetrahedral with bond angle 109° . But oxygen atom contains two lone pairs of electrons. It causes repulsion between bond pair leading to decrease in bond angle to 104° . Therefore water molecule shows bent shaped or distorted tetrahedral shape.

Aluminium chloride shows trigonal planar geometry with 120° bond angle. Aluminium forms three bonds with chlorine atoms and it is not having any lone pair of electrons hence it shows trigonal geometry whereas in Phosphorous trichloride phosphorus contains a lone pair of electron. In PCl_3

there is repulsions between lone pair and bond pair and hence it changes from trigonal planar to shows trigonal pyramidal geometry with bond angle 104° .

In phosphorus pentachloride, phosphorus is bonded to five chlorine atoms. It shows trigonal bipyramidal geometry. In this molecule axial bonds are longer forming 90° bond angle and equatorial bonds are shorter with 120° bond angle. In this molecule chlorine atoms repel each other and so the shape of the molecule is trigonal bipyramidal causing minimum repulsion between atoms in a molecule.

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. The geometry and shape of a molecule is defined by the bond pair-bond pair or lone pair-bond pair or lone pair-lone pair interactions in a molecule as explained with the help of VSEPR theory. These interactions also contribute to the reactivity of molecules. A molecule with minimum repulsions is most stable whereas more the repulsions in a molecule makes it highly unstable, making molecule highly reactive.

Reference:

[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.](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)