

Drawing Single atoms:

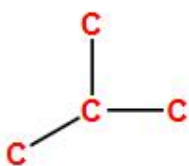
1. Select any of the atom buttons below by clicking them or click periodic table button on the rightmost of the toolbar to select the atom of your choice.



2. Click on the drawing area below the toolbar to draw the atom.

Drawing bonded atoms:

1. Select the corresponding atom by clicking on the atom buttons.
2. Click and drag on the drawing area to form two atoms with single bond between them.
3. To form a bond with already present atom on the drawing area, click and drag on the corresponding atom.

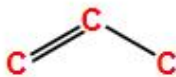


Drawing double & triple bonds:

There are two ways to draw double or triple bonds

Option 1:

1. Select the corresponding atom by clicking on the atom buttons.
2. Click and drag on the drawing area to form two atoms with single bond between them.
3. Again click and drag on the same atoms to form another bond.



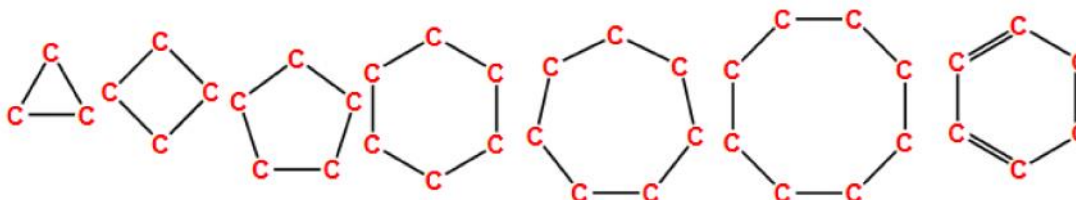
Option 2:

1. Select the corresponding bond skeleton button mentioned in below image.
2. Click and drag between the two atoms to convert them into corresponding bond.



Drawing ring fragments:

1. Select the corresponding ring from toolbar.
2. Click and drag on the drawing area to form the ring in the corresponding orientation.



Drawing bridge fragments:

1. Select the corresponding bridge from toolbar.



2. The number of the bridge denotes the number of atoms in the bridge.
3. Click on the start atom of the bridge and drag drop to create the next member in the bridge.
4. Connect the bridge with last atom to complete the bridge else the temporary bridge formed will be erased.



Temporary One Member Bridge



Completed One Member Bridge

Show/Hide Grids:

Grid is provided for better aligning of the atoms.

1. Click on the grid to activate them. Click again on them to deactivate it.

Show/Hide Implicit Carbon:

Carbon once filled with its valency it becomes implicit and are hidden.

1. Click on the implicit carbon button to show them. Click again on them to hide them.

Undo/Redo:

Undo and redo are provided to correct unintended mistakes.

1. Click on the undo button to undo or use keyboard shortcut ctrl+z.
2. Click on the redo button to redo or use keyboard shortcut ctrl+y.

Delete Structure:

Entire structure can be deleted with this option

1. Click on the delete structure button and click on any atom of the structure to delete the entire structure completely.

Erase Arrow/Sign:

Arrows(direct & reversible) and signs can be deleted with this option

1. Click on the erase arrow/sign button and click on any arrow/sign to erase it.

Move Structure Group:

The entire structure group can be moved with this option

1. Click on the move structure group button and click on any atom on the drawing area, drag and place them wherever required.

Move Structure:

The entire structure can be moved with this option

1. Click on the move structure button and click on any atom of the structure on the drawing area, drag and place them wherever required.

Move Atom:

The entire atom can be moved with this option

1. Click on the move atom button and click on the corresponding atom, drag and place them wherever required.

Above Plane Projection:

The bond can be represented to show it above the drawing plane using this option

1. Click on the above plane projection button and click on any bond that must be represented above the plane.

Below Plane Projection:

The bond can be represented to show it below the drawing plane using this option

1. Click on the below plane projection button and click on any bond that must be represented below the plane.

In Plane Projection:

Any bond represented above/below the plane can be brought back to current plane using this option

1. Click on the in plane projection button and click on any bond that must be represented in line with the plane.

Change Orientation:

The atom's orientation can be changed with this option

1. Click on the change orientation button and click on any atom and drag around to change its orientation (only the target atom's orientation can be changed).

Show/Hide Unpaired Electrons:

The unpaired electrons in an atom can be shown or hidden with this option

1. Click on the show/hide unpaired electron button and to view unpaired electrons of atoms in the drawing area. Click again on the button to hide the unpaired electrons.

Show/Hide Lone pair of Electrons:

The lone pair of electrons in an atom can be shown or hidden with this option

1. Click on the show/hide lone pair of electron button and to view lone pair of electrons of atoms in the drawing area. Click again on the button to hide the lone pair of electrons.

Show/Hide Vacant orbitals:

The vacant orbitals in an atom can be shown or hidden with this option

1. Click on the show/hide vacant orbital button and to view vacant orbital of atoms in the drawing area. Click again on the button to hide the vacant orbitals.

Atom Position Numbering:

The atom position in a structure can be represented with this option

1. Click on the atom position numbering button and click on an atom and enter the position number in the input prompt.

Isotopic Labeling:

The isotope of an atom can be represented with this option

1. Click on the atom isotope labeling button and click on an atom and select the isotope value from the dialog box.

Add Charge:

The charge on an atom can be represented with this option

1. Click on the add charge button and click on an atom and select the charge value from the dialog box.

Ion-Ion Interaction:

The interaction between two ions of opposite charges can be represented with this option

1. Click on the ion-ion interaction button and click and drag between the two ions to draw the interaction between the two ions.

Ion-dipole Interaction:

The interaction between ion and dipole of opposite charges can be represented with this option

1. Click on the ion-dipole interaction button and click and drag between the ion and dipole to draw the interaction between the two ions.

Dipole-dipole Interaction:

The interaction between two dipoles of opposite charges can be represented with this option

1. Click on the dipole-dipole interaction button and click and drag between the two dipoles to draw the interaction between the two dipoles.

Hydrogen Bonding Interaction:

The interaction between a hydrogen atom and an ion can be represented with this option

1. Click on the hydrogen bonding interaction button and click and drag between the hydrogen atom and an ion to draw the hydrogen bonding interaction.

Draw Arrow:

An ordinary arrow can be drawn with this option

1. Click on the draw arrow button and click and drag to draw the arrow at the respective position.

Draw Reversible Arrow:

A reversible arrow can be drawn with this option

1. Click on the draw reversible arrow button and click and drag to draw the reversible arrow at the respective position.

Draw Plus Sign:

A plus sign can be drawn with this option

1. Click on the draw plus sign button and click on the respective position to draw the plus sign.

Draw Minus Sign:

A minus sign can be drawn with this option

1. Click on the draw minus sign button and click on the respective position to draw the minus sign.

Show XML:

Click on the show XML button to view the XML generated for the corresponding structures on the drawing area.

File Menu:

Hover over the file menu to view the options provided.

1. New option is to clear the drawing space.
2. Open option is to open an XML file already generated through save option.
3. Open template option is to reuse template file saved through save template option.
4. Save option is to save the structures as an XML output.
5. Save Image option is to generate image file in png format.
6. Save template option is to save single structure as template and reuse it again through open template.

Caption Menu:

Hover over the caption menu to view the options provided.

1. Add caption – Click on the drawing area where caption must be added and enter the caption name in the prompt that follows.
2. Move caption – Click on the caption and drag it to move across the drawing space.
3. Delete caption – Click on the caption to delete it.

Template Menu:

Hover over the caption menu to view the options provided.

1. Show library – An in-built library containing some template frequently used are present. Select one of the templates from the dialog box and click on the drawing area to draw the respective template on that point.
2. Update library – Logged in users can update the library by adding their own templates to the in-built library.