

Draw structures

MolDraw Docs · LabCanvas · 9 pages · mol draw.com/docs/

Draw atoms

Short answer: Pick an element in the atom palette, then click the canvas or the end of a bond. Click an atom to change it. Use the periodic table for other elements.

- 1 Click an element in the atom palette, for example **N**.
- 2 Click an empty spot to place it. Or click an atom to change it.
- 3 For other elements, click the grid button and pick from the periodic table.

Keyboard tricks

- With nothing selected, press a letter like **N** or **O** to set the element.
- With one atom selected, type a symbol to rename it. Type **Cl** or **Br** for two letters.
- Type groups like **Me**, **Ph** or **OMe** too.

Change an atom

Right click an atom. You can set the element, isotope, charge, explicit H, lone pairs and radicals.

TIP

The **A** button places an "any atom". It is the same as ***** in SMILES.

Questions and answers

How do I add a chlorine atom?

How do I add an isotope like deuterium?

Source: <https://www.mol draw.com/docs/drawing/how-to-draw-atoms-and-change-elements/>

Draw bonds

Short answer: Pick a bond type in the left rail and drag from atom to atom. Click a bond to change its type. Press 1, 2 or 3 for single, double or triple bonds.

- 1 Click the bond button in the left rail. Open the small arrow for more types.
- 2 Drag from an atom to draw a bond. Or click an atom to grow a bond from it.
- 3 Click an existing bond to switch it to the chosen type.

Bond types

Single, double, triple, aromatic, wedge, hash, wavy, bold, dative, hydrogen bond (dotted), cis/trans, any and centroid bonds are all in the bond menu.

Shortcuts

- **1** single, **2** double, **3** triple.
- **B** benzene ring.

TIP

The **Chain** tool draws a zigzag chain in one drag. Watch the count as you drag.

Questions and answers

How do I draw a double bond?

How do I draw a wedge bond?

Source: <https://www.moldraw.com/docs/drawing/how-to-draw-single-double-triple-and-wedge-bonds/>

Rings and structures

Short answer: Use the ring bar at the bottom to place rings from 3 to 8 atoms. Click a ring atom or bond to fuse a new ring. Clean up tidies the shape.

- 1 Click a ring in the ring bar, such as benzene or cyclohexane.
- 2 Click empty canvas to place it.
- 3 Click an atom or bond of a ring to fuse or attach another ring.
- 4 Click **Clean up** to even out bonds and angles.

Special rings

- The small arrow under cyclohexane gives chair and boat shapes.
- The arrow under benzene gives a tilted arene for metal complexes.
- Cyclopentadiene has a Cp option.

Select and move

Drag a box with the select tool. Hold **Shift** and drag for a lasso. Use the handles to rotate or resize.

NOTE

For ChemDraw style ring shapes, turn on Indigo layout in **Settings**.

Questions and answers

How do I draw naphthalene?

How do I draw a chair cyclohexane?

Source: <https://www.moldraw.com/docs/drawing/how-to-draw-benzene-cyclohexane-and-fused-rings/>

Atom labels and R-groups

Short answer: Pick the atom label tool (A) and click an atom. Type a label like Ph, COOH or R1. MolDraw can expand known labels into full structures.

- 1 Click the **Atom label** tool in the left rail.
- 2 Click an atom.
- 3 Type a label, such as `Ph` , `COOH` , `Boc` or `R1` .
- 4 Press `Enter` .

Expand or collapse a label

Right click a label. Pick **Expand** to show every atom. Pick **Collapse** to go back to the short label.

TIP

Labels MolDraw does not know stay as text. They still show on your figure.

Questions and answers

How do I add an R group?

Source: <https://www.moldraw.com/docs/drawing/how-to-add-atom-labels-and-r-groups/>

Stereochemistry

Short answer: Use wedge and hash bonds for 3D centers. Open Chemistry and pick Show CIP labels to see R and S. Right click to invert a center.

- 1 Pick **Wedge up** or **Hash down** in the bond menu.
- 2 Drag from the stereo center to the outer atom.
- 3 Open **Chemistry** and click **Show CIP labels** to see R, S, E and Z.

More stereo tools

Right click a suitable atom, bond or ring. You can invert a center or make Newman, Fischer, chair and boat views.

WARNING

Wedges point away from the stereo center. Draw from the center outward.

Questions and answers

How do I show R and S labels?

How do I flip a stereocenter?

Source: <https://www.moldraw.com/docs/drawing/how-to-draw-stereochemistry-wedge-hash-and-r-s-labels/>

Lone pairs, radicals and charges

Short answer: Pick the lone pair tool and click an atom to add a pair of dots. Use the radical tool for one dot. Charge tools add plus and minus marks you can drag around the atom.

- 1 Click the **Lone pair** tool in the left rail.
- 2 Click an atom. A pair of dots appears.
- 3 Drag the dots around the atom to a free side.
- 4 For a radical, open the small arrow and pick the radical tool.

Charges

Use + and - in the rail. Click again for +2 or -2. The rail also has circled charges and $\delta+$ and $\delta-$.

When to show lone pairs

Show lone pairs when you draw mechanisms. A curved arrow should start at a lone pair or a bond. Oxygen in water has two pairs. Nitrogen in ammonia has one.

TIP

Check that charges match electrons. Oxygen with three bonds and one lone pair is +1.

Questions and answers

How do I add a lone pair in MolDraw?

How do I add a radical?

Source: <https://www.moldraw.com/docs/drawing/how-to-add-lone-pairs-radicals-and-formal-charges/>

Polymer brackets

Short answer: Select the repeat unit, then click the Brackets tool. Click the small n to change the number of units.

- 1 Select two or more atoms of the repeat unit.
- 2 Click **Brackets** in the left rail.
- 3 Click the subscript to type n, m or a number.

Click Brackets again for more types. You get polymer n, copolymer m and parenthesis (CH₂)n. Brackets move with the structure.

Questions and answers

How do I draw a polymer repeat unit?

Source: <https://www.moldraw.com/docs/drawing/how-to-draw-polymer-repeat-unit-brackets/>

Text, shapes and images

Short answer: Open the Draw ribbon to add text, shapes, images and glassware. Click the canvas to place them and drag to move.

Add text

- 1 Click the **Text** button (T) in the tools row.
- 2 Click empty canvas and type.
- 3 Press **Esc** when you are done.

Shapes, images and glassware

- **Shapes** gives arrows, boxes and outlines.
- **Image** adds PNG, JPEG, WebP, GIF or SVG files.
- **Glassware** adds lab apparatus. You can set a liquid level.

Questions and answers

Can I add lab glassware to my figure?

Source: <https://www.moldraw.com/docs/drawing/how-to-add-text-shapes-images-and-lab-glassware/>

Style and display

Short answer: Open Color and style to change colors, font, bond width and the structure look. Settings control hydrogens, labels, grid and snap.

- 1 Select what you want to change, or nothing for the whole drawing.
- 2 Click **Color and style** in the tools row.
- 3 Pick colors, label style or the **Look**, such as Ball and stick.

Settings

Click **Settings** (gear). You can change implicit hydrogens, colored atom labels, grid and snap. You can also save style presets.

TIP

For ACS style in a paper, pick a style preset in Settings, then export SVG.

Questions and answers

How do I color an atom?

Source: <https://www.moldraw.com/docs/drawing/how-to-change-structure-style-colors-and-display/>