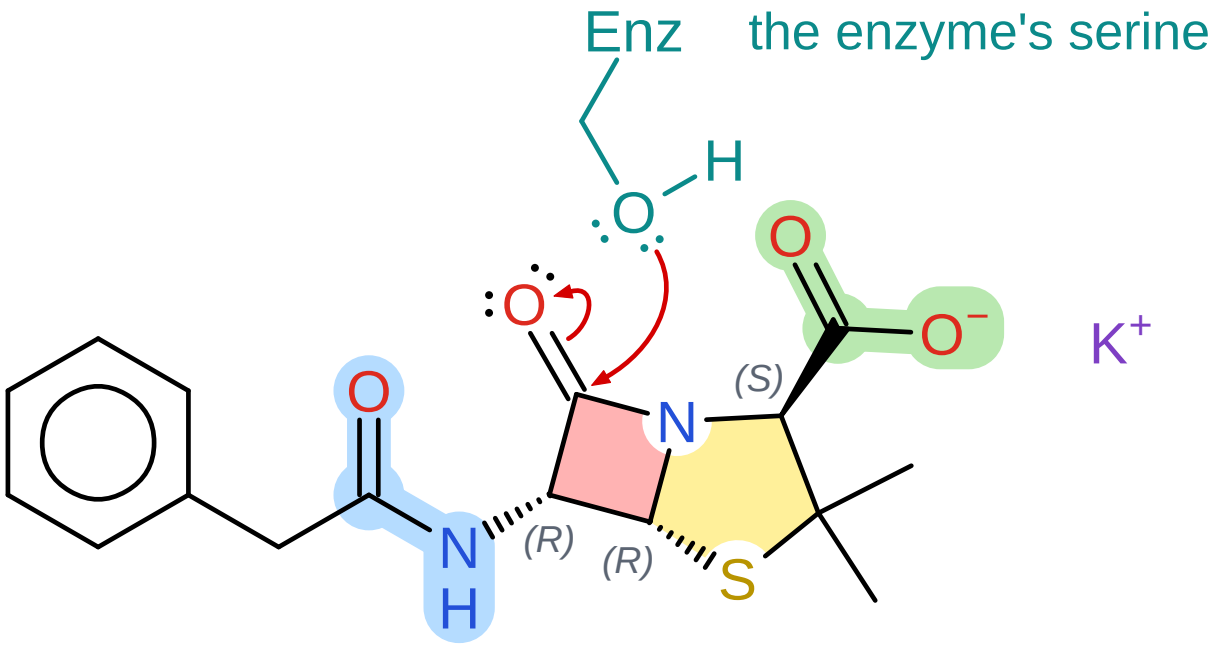
olomol

Manual

Drawing chemical structures, reactions and mechanisms in the browser



curved arrows · lone pairs · wedges and R/S · ring fills · highlighting · colours · charges · aromatic circle · group labels · text

Jan Salomon
Department of Physical Chemistry, Palacký University Olomouc

testing version · November 2026

Contents

1 Introduction 1
1.1 What olomol is 1
1.2 Opening 1
1.3 The window 2
1.4 Help and examples 2
1.5 The drawing saves itself 3
1.6 Moving and zooming 3
2 Drawing structures 4
2.1 Bonds and atoms 4
2.2 Chains and rings 4
2.3 Elements, the periodic table and group labels 4
2.4 Charges, radicals and hydrogens 5
2.5 Stereochemistry 6
2.6 Special bonds 6
2.7 Selecting, moving, rotating and deleting 6
2.8 Keeping particles together 7
2.9 Copying and pasting 7
2.10 Text 7
2.11 Reaction arrows 7
2.12 Anchors 8
2.13 Side arcs on reaction arrows 8
2.14 The panel on the right 9
3 Templates and structures from names 10
3.1 Searching 10
3.2 Functional groups attach 11
3.3 Conformations and projections 11
3.4 Complexes 12
3.5 Structures from a name or SMILES 12
4 Mechanisms 14
4.1 Lone pairs and unpaired electrons 14
4.2 Curved arrows and fishhooks 14
4.3 When an arrow does not look right 15
4.4 Orbitals 15
4.5 Resonance structures, transition states and brackets 16
4.6 Aromatic rings 16
5 Editing and arranging 17
5.1 Redraw 17
5.2 Turn in 3D 17
5.3 Redrawing only a part 19
5.4 Align and grid 20
5.5 Flipping and straightening 20
6 Atom numbering and the Info card 22
6.1 IUPAC numbering 22
6.2 Your own numbers 22
6.3 The Info card 22
6.4 Finding a compound on PubChem 22
7 Colours and highlighting 24
7.1 Colour 24
7.2 Highlighting and filled rings 24
7.3 Example: what molecules have in common 24
8 Files, export and links 26
8.1 Save and open 26
8.2 Exporting pictures and files 26
8.3 Into Word, PowerPoint and Google Docs 27
8.4 Links 27
9 Settings and keyboard shortcuts 28
9.1 The look of the drawing, language and window 28
9.2 Keyboard shortcuts 28
10 Installing, limitations and reporting problems 30
10.1 Installing as an app and working offline 30
10.2 Known limitations 30
10.3 Problems and ideas 30
A How olomol is built 32
A.1 The big picture 32
A.2 What each part does 32
A.3 Rules that are not from the libraries 33
A.4 Data and files 33
A.5 What leaves the computer 33
A.6 Offline and installing 33
A.7 Development and tests 33
A.8 Licence and credits 34

1 CHAPTER Introduction

This manual shows you how to do what you need when drawing chemistry: draw a molecule or a mechanism with curved arrows, arrange it neatly, and get it into Word, PowerPoint or Inkscape. The chapters follow tasks rather than buttons, so you can go straight to the one you need. If you are new to the program, start with the short *Quick start*. If you would like to know how it works inside, see the appendix (appendix A).

Names of buttons and menus are written like this and match exactly what you see on the screen when the program is in English. Keys look like this: `Ctrl+Z`. On a Mac, use `Cmd` instead of `Ctrl`.

1.1 What olomol is

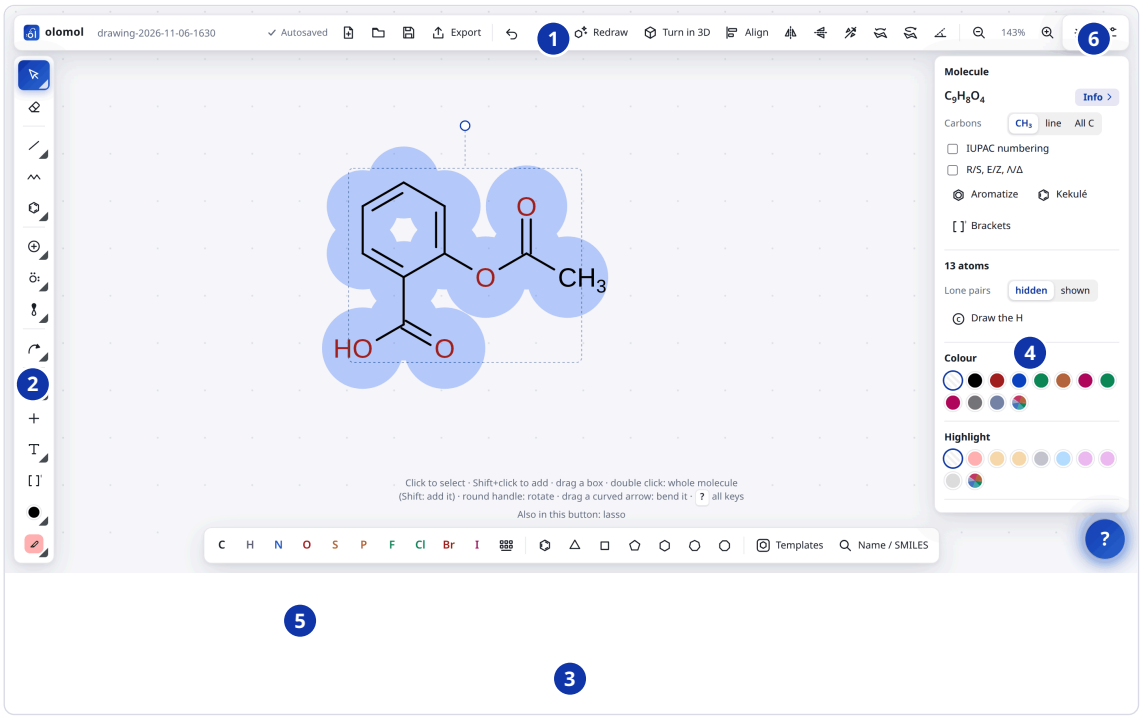
olomol is a free chemistry drawing program that runs entirely in your web browser. It was made for teaching, as a replacement for ChemSketch. It draws structures, reaction schemes and mechanisms with lone pairs and curved arrows, and it exports clean pictures for lab reports, theses and presentations.

- **Nothing to install.** Chrome, Edge or Firefox is enough, on Windows, Mac or Linux. If you prefer, you can install it as an app (section 10.1).
- **Your drawings stay with you.** The program has no accounts and no server that stores drawings. Something leaves your computer only when you ask for it: looking up a name in PubChem sends the name you typed, and a link to a drawing carries the drawing inside it.
- **The chemistry is real.** The program knows how many hydrogens and lone pairs an atom has, computes the formula, masses and identifiers, and makes sure that tidying a drawing never changes the molecule behind your back. The RDKit, Indigo and OpenChemLib libraries do this work on your own computer.

1.2 Opening

The first visit takes a little longer, and a bar shows how much is left. The chemistry libraries are downloaded only when they are first needed (you may see Loading the chemistry engine (RDKit)…). After that they stay on your computer, and the program works without the internet too.

1.3 The window



1. **Top bar**: the drawing's name, new drawing, open, save, Export, undo and redo, Redraw, Turn in 3D, Align, flips, ring flip and turning a chair, Horizontal / vertical and zoom.
2. **Drawing tools.** A small triangle in a button's corner means it has more variants: rest the pointer on the button, click the triangle, or click the chosen tool again.
3. **Bottom bar**: elements, the periodic table, rings, Templates and Name / SMILES.
4. **Panel** with the properties of whatever is selected (section 2.14).
5. **Hints** for the chosen tool. The ? key shows all keyboard shortcuts.
6. Reporting a problem (section 10.3) and settings: the look of the drawing, the language, the theme and debug mode (chapter 9).

1.4 Help and examples

Rest the pointer on any button and a tooltip tells you what it does, along with its shortcut. The hint line at the bottom changes with the chosen tool, so it is worth a glance whenever a tool surprises you. Below it, a second line names what else the tool's button holds (behind the small corner of the button): the bond tool's wedges, dative and hydrogen bonds, say. Where the top bar has room, its buttons have words as well; in a narrower window they drop them, Turn in 3D's first.

The round button ? at the bottom right opens **Help**, the quickest way to see how something is done. It holds more than twenty finished drawings, shown as small pictures. Tags such as Mechanisms, Stereochemistry or Texts narrow the list down.

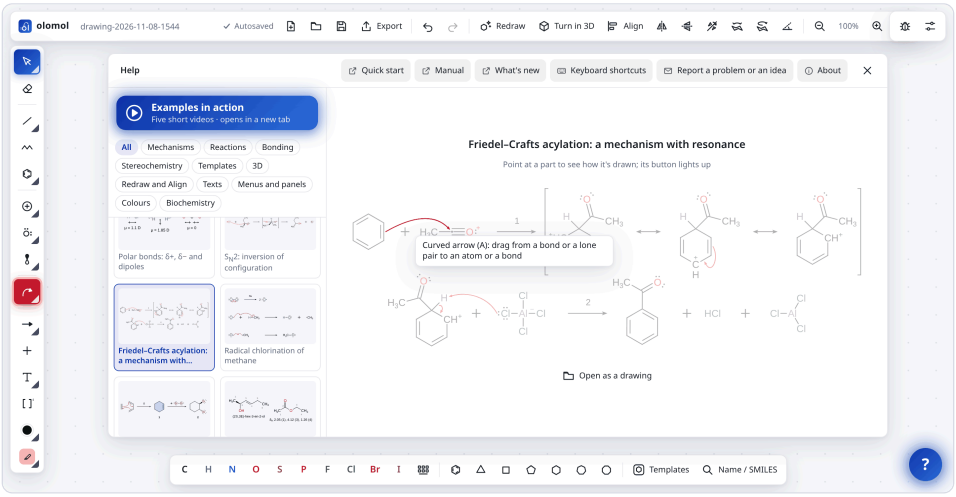


Fig. 1: Help: pointing at a curved arrow says how it is drawn, and its button lights up in the left bar

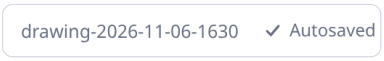
- Pick an example and **point at any part of it**: a tip says how that part is drawn, and the button you would use lights up in the program's bars.
- What cannot be shown by pointing (Redraw, Templates, Align) is listed as steps under the drawing.
- Open as a drawing makes the example your own, to look at closely or to change. Ctrl+Z brings back what you had before.

Above the tags, Examples in action opens the about page in a new tab, with five short videos of olomol at work: a mechanism, a reaction scheme, a molecule built in steps and partly redrawn, a complex turned in 3D, and a Haworth projection of glucose made a chair, flipped and turned in 3D.

The header of the Help window has the Quick start and this Manual (PDF; the Czech ones when the program is in Czech), What's new with the changes in each version, Keyboard shortcuts, Report a problem or an idea (section 10.3, also the bug at the top right) and About, with the credits and licences. What's new and About are also under the version in the bottom left corner.

1.5 The drawing saves itself

You need not worry about losing your drawing. The browser remembers it by itself, a moment after each change, so you can close the window or turn off the computer and it will be waiting when you come back. The mark beside the drawing's name shows this: Autosaving… just after a change, then Autosaved.



This covers one drawing, the one on the canvas, in this browser on this computer. To have several drawings, to move one to another computer or to send it to someone, save it as a file with Save (Ctrl+S, chapter 8). A file is also the safest home for work that matters to you, because it stays even if the browser's data are cleared.

The mark warns you in two cases. Not autosaved means this browser can't autosave, as in a private window or when its storage is full: save your drawing to a file before you close it. Another tab means olomol is open in a second tab that has autosaved its own drawing since. Next time, the one changed last comes back, so save this one if you want to be sure of it.

The button starts a new drawing on an empty canvas, and Ctrl+Z brings the previous one back. The empty canvas shows a faint example, a different one of four each time. Point at a part of it to learn how it is drawn, and its button lights up in red.

At the top left, next to the logo, is the **drawing's name**. It starts as `drawing-` with the date and time, so files do not overwrite each other. Click it to rename the drawing; saved files are named after it.

1.6 Moving and zooming

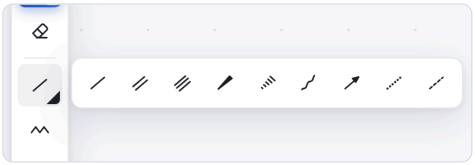
To zoom, use Ctrl + wheel or the magnifiers at the top. The percentage between them returns to 100 %. The button shows the whole drawing; with something selected, it centres the selection and zooms in until it fills the window. **To move the canvas**, use the wheel (with Shift for sideways), drag with the space bar held down, or drag with the middle mouse button.

2 CHAPTER Drawing structures

2.1 Bonds and atoms

Everything starts with the single bond (/), which is already chosen when the program opens.

- **Click the empty canvas:** the first bond appears.
- **Click an atom:** a new bond grows from it. The program picks a sensible direction, zigzag and into the largest gap; a chain runs across the page. With Shift the bond goes to the other side (the next best place), so a chain can bend the other way.
- **Drag from an atom:** pull a bond where you want it, in 15° steps, or at any angle with Shift. Release it on another atom to close a ring. Over the target atom the bond snaps straight to it, so you see the result at once.
- **Click a bond:** it changes from single to double to triple.



The other kinds of bonds are among the tool's variants (in the picture, from the left): single, double, triple, wedge, hashed wedge, wavy, coordination, hydrogen and partial bond. Clicking a double bond with the double bond tool moves its second line to the other side or to the middle. Clicking a wedge with the wedge tool turns it round.

You can also work from the keyboard without switching tools. Point at a bond and press 1, 2 or 3. Pressing 1 again over a single bond makes it a wedge, then a hashed wedge, then both from the other end, and then a plain bond again. Shift+1 goes through them backwards.

2.2 Chains and rings

The chain tool (Z) draws a zigzag chain: drag from an atom or from the canvas. While you drag, it shows how many bonds it adds; with Shift the zigzag starts the other way.

Rings are in the bottom bar (benzene and 3- to 8-membered rings) and among the variants of the ring tool on the left. Before you click, a see-through preview shows what will happen:

- clicking the **canvas** draws a ring on its own,
- clicking a **bond** adds a fused ring (naphthalene from benzene), with Shift on the bond's other side,
- clicking an **atom** attaches the ring by a new bond (phenyl); dragging from the atom aims it,
- clicking an atom with Shift puts the ring through that atom (a spiro compound).

2.3 Elements, the periodic table and group labels

The bottom bar has the most common elements, each in its own colour so you find them quickly. Pick one, and then:

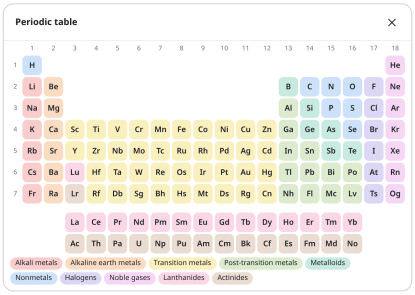
- **click an atom** to change it to that element,
- **click an atom that already is that element**, or any atom with Shift, to bond a **new atom** of the element to it (clicking carbon on carbon extends a chain),
- **click the canvas** to put down a lone atom (O: water),
- **drag from an atom** to draw a bond to a new atom.

The element keys are quicker: C N O S P F H I, with L for Cl and B for Br. What a key does depends on where the pointer is.

- **Over an atom**, the atom becomes that element, once, and your tool stays as it was.
- **Over empty space**, you start **drawing with that element**. It lights up in the bottom bar and works just as described above. Clicking a bond still changes the bond, and 1 2 3 set the order of new bonds while the element stays (N, then 2: a double bond to N). C switches back to carbon.

This way you can draw with heteroatoms straight away, instead of drawing a carbon skeleton and rewriting it afterwards.

The ⊞ button after the elements opens the Periodic table. Its elements are coloured by group (Alkali metals, Halogens, Noble gases…) and carry group and period numbers.



Group labels and abbreviations are in Templates → Abbreviations and attach like functional groups (section 3.2):

- **Placeholders** such as R, R′, X, Nu, E, LG or Ar have no hydrogens or lone pairs, which suits general mechanisms. (Ar here is aryl, not argon.)
- **Abbreviations** such as Me, Et, Ph, Bn, Ac, Boc, Ts, OMe or CO2Et count in the formula and mass, and files get the whole group. To the left of a bond they are written reversed (MeO–, EtO2C–).

With an atom selected, you can also type an abbreviation or a placeholder into the Element field of the panel. An isotope is written with its mass number (13C, 18O), and deuterium and tritium as D and T, or 2H and 3H. A symbol is taken as written (Cl, Na) or all in small letters (cl, na); CO or NI is refused rather than read as cobalt or nickel, since two capitals are two atoms.

Draw out in the panel draws the group an abbreviation stands for (Ph as a benzene ring), and Abbreviate does the opposite for a selected group. A wedge on the bond to the group stays, so the stereochemistry does not change. An abbreviation stands for a group on one bond, so it takes no second one: draw it out first to bond to its atoms. Charged groups have abbreviations too, with the charge on the label: SO_3^- (a sulfonate), CO_2^- or COO^- (a carboxylate), OPO_3^{2-} and OPO_3H^- (phosphates) and PO_3^{2-} drawn out, the charge sits on an O, where it belongs.

2.4 Charges, radicals and hydrogens

The charge tool on the left has four kinds: positive ⊕, negative ⊖ and the partial charges **δ+** δ+ and **δ–** δ−. Click an atom, and click again to raise the charge (or lower it, with the negative one); a partial charge clicked again goes. + and − choose the positive and the negative one.

The unpaired electron c• is a variant of the lone pairs tool ö:. Click an atom for one electron, again for two side by side (a singlet), and again for none. Two on separate sides (a triplet), three or four are in the panel's Unpaired row; on an atom without bonds its lone pairs show with them, as a Lewis symbol (·N̈·).

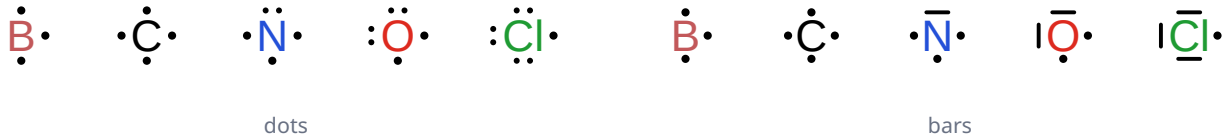


Fig. 5: Lewis symbols of B, C, N, O and Cl, in dots and in bars (Settings → Lone pairs)

Over an atom you can also press + or − for a charge and . for an unpaired electron.

Other keyboard layouts Digits are read by the key's position, so 1 2 3 also work in the top row of a Czech keyboard, for example (+ ě š). Over an atom, the + in that row raises its charge; over empty space it acts as 1, so choose the positive charge tool with + on the number pad, or with its button ⊕.

An atom with more bonds than it can have gets a **red dashed ring**, which shows only on screen and never in pictures. The panel then says what is wrong, for example Si can't have 6 bonds. Usually a charge is missing; for SiF_6^{2-} see section 3.4.

Hydrogens are worked out from the bonds and the charge (CH_3, NH_2, OH). To set another number, use the Hydrogens row of the panel. Draw the H draws the hydrogens of the selected atoms as atoms of their own, which you need when a curved arrow goes to or from a hydrogen. Hide drawn H hides them again.

Chain ends are written as CH_3 by default. The Carbons switch in the panel (CH_3, line or All C) changes this for the selected carbons: the whole molecule, or just one end. All C writes every carbon (CH_3, CH_2, CH), for those who do not yet read a corner as a carbon. The default for new drawings is in Settings.

2.5 Stereochemistry

The wedge points towards you and the hashed wedge away from you. Both are among the bond tool's variants. A wedge starts at the atom you drag from, so its narrow end is at the stereocentre. The wavy bond marks an undefined configuration.

To show **R/S and E/Z** labels (Λ and Δ for complexes), tick R/S, E/Z, Λ/Δ in the panel, for the whole selected molecule or just the selected atoms and bonds. RDKit computes them, and they also go into exported pictures and KET files.

When a bond joins the wide ends of two wedges it is drawn bold, as is customary (the bridge of a morphinan, the front edge of a Haworth formula).

2.6 Special bonds

The bond tool's variants also include three bonds that do not count like ordinary ones. The key D chooses the first of them, and each further press the next (over a bond, it turns that bond into them):

- a **coordination (dative) bond**, an arrow from the donor, which spends a lone pair on it (another click turns it round),
- a **hydrogen bond**, drawn dotted,
- a **partial bond**, forming or breaking, drawn dashed, for transition states.

A wedge or a hashed wedge gives a coordination bond depth, with its narrow end at the metal, and it stays a coordination bond, so the donor gets no extra bond. Redraw and Turn in 3D then keep the mirror image (Λ or Δ) you drew: Redraw does not offer drawings that would lose it, and Turn in 3D warns at a view that would. For an octahedral complex with two or three chelates (cis-$[CoCl_2(en)_2]^+$, $[Co(en)_3]^{3+}$), R/S, E/Z, Λ/Δ writes (Λ) or (Δ) beside the metal. If you prefer, Settings can draw these arrows as plain lines.

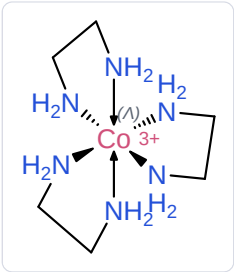


Fig. 6: $[Co(en)_3]^{3+}$ drawn with wedges; R/S, E/Z, Λ/Δ writes (Λ) or (Δ) beside the metal

These bonds are kept in KET files and pictures, but not in molfile, SMILES and similar files (section 10.2).

2.7 Selecting, moving, rotating and deleting

The Select tool (V, or Esc) does the following:

- a click selects an atom, bond, arrow or text, and Shift+click adds to the selection,
- dragging over empty space selects everything in a box; the tool's variants include a lasso, and Esc switches between the two when there is nothing left to cancel,
- a **double click** selects the whole molecule, Shift+double click adds it to the selection, and Ctrl+A selects everything,
- dragging moves the selection, and so do the arrow keys (with Shift, further),
- the **round handle** above the selection rotates it,
- an atom or bond dragged onto another atom **merges** with it. It snaps while you drag and shows the result; drag on and it lets go. A filled ring keeps its colour as long as it stays a ring.

To delete, use the eraser (E), which works by clicking or with a box. Delete or Delete in the panel removes the selection. With nothing selected, Delete removes whatever is under the pointer.

Every step can be undone, so feel free to try things: Ctrl+Z undoes and Ctrl+Shift+Z redoes.

2.8 Keeping particles together

A salt such as K_2SiF_6 is three separate particles (K^+, K^+ and SiF_6^{2-}). Select them all and click **Keep together** in the panel. An invisible link joins them, so they move, align and go into a grid as one molecule, and the panel shows one formula (F_6K_2Si).

The links show while the group is selected, or all the time when **Links** in **Settings** is set to **shown**. **Keep apart** separates the particles again. Links are not written to molfile and SMILES.

2.9 Copying and pasting

`Ctrl+C`, `Ctrl+X` and `Ctrl+V` work as they do elsewhere. A pasted copy follows the pointer, see-through, until a click puts it down, and `Esc` cancels.

You can paste from elsewhere too: a SMILES, InChI or molfile copied from a web page or another program is drawn straight away with `Ctrl+V`. A double bond whose E or Z the SMILES leaves open gets a wavy bond beside it.

2.10 Text

Choose the text tool `T` (`T`), click and type. What you type stays exactly as written, so the numbers in a DOI or a name are left alone. A bar over the text holds everything for formatting it:

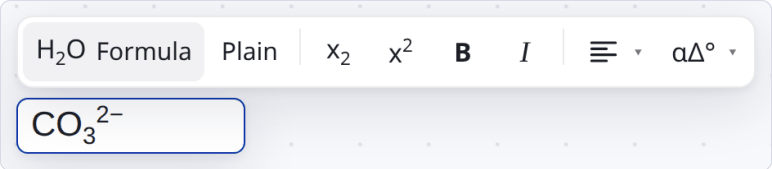


Fig. 7: The bar over a text, after **Formula** turned CO32- into a formula

- **Formula** turns the selected part, or with nothing selected the whole text, into a formula. Digits after letters become subscripts and a charge at the end (Fe3+, CO32-, [SiF6]2-) a superscript. It also understands CO_3^2-, and e- or 2e- as the electron's charge. **Plain** removes the formatting.
- What this rule cannot do, you set by hand: x_2 (`Ctrl+,`), x^2 (`Ctrl+.`), **B** (`Ctrl+B`) and *I* (`Ctrl+I`). They change the selected part or, with nothing selected, what you type next.
- The bar's menus hold the alignment of lines (a multi-line text under a molecule or on an arrow is otherwise centred) and special characters: Greek letters, arrows, °, ±, ‡.

`Enter` finishes the text and `Shift+Enter` starts a new line. A copied text reaches other programs as plain words, so a DOI pastes straight into the browser.

2.11 Reaction arrows

Choose the reaction arrow → (`X`). A click puts down an arrow of standard length, and dragging draws your own (`Shift`: at any angle). Its variants are equilibrium ⇌, resonance ↔, retrosynthetic ⇒, multi-step ⇉, crossed ↠ (a reaction that does not go), the equals sign = (the same thing drawn another way, a chair = its Haworth projection; **Align reaction scheme** spaces it like an arrow) and the dipole arrow ↦, which moves with its molecule. To change a selected arrow's length, use **Length** in the panel (in bond lengths) or drag its end.

For an equilibrium that lies to one side, select the equilibrium arrow and click the button in the panel's **Favours** row: each click moves it on, from even to the products' side (the lower harpoon shorter) and to the reactants' side (the upper one shorter).

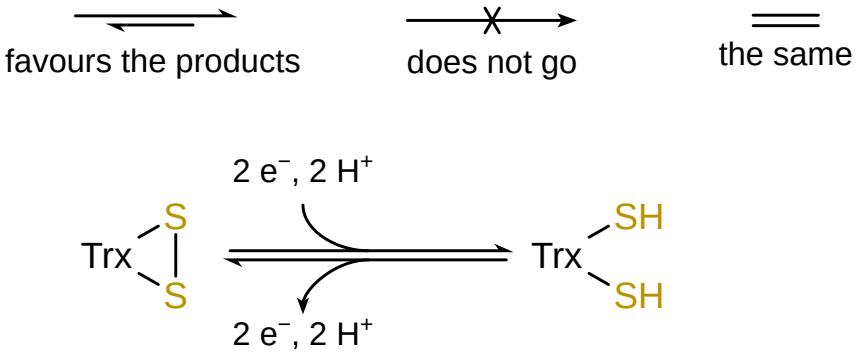


Fig. 8: Top, an equilibrium that favours the products, the crossed arrow and the equals sign. Below, thioredoxin reduced: 2 e^- and 2 H^+ come in on the upper harpoon's arc and leave on the lower one's on the way back

The ⊕ tool puts a plus sign between reactants.

2.12 Anchors

Anchors keep a text or a reagent with whatever it belongs to, so you never have to move things one by one.

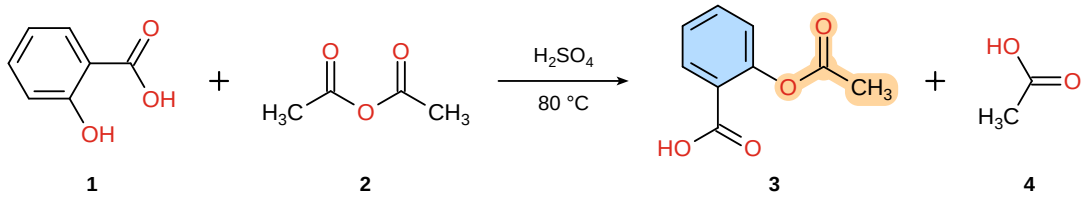


Fig. 9: A reaction scheme with compound numbers on the anchors under the molecules

On a molecule. Every molecule has four places for text: below, above, left and right. Drag a text towards a molecule and the anchors show as boxes, with the nearest one highlighted. Release, and the text stays there: it now moves and aligns with the molecule. Several texts on one anchor stack up, and dragging one to another place changes the order. This is how you put a compound number under a molecule or a count (2 NaOH) to its left. In the panel, the arrow buttons ↓ ↑ ← → choose the anchor and free frees the text; dragging it away from the molecule frees it too. A text you type right under, over or beside a molecule goes on that anchor at once.

On a reaction arrow. An arrow has anchors above and below. Drag a text (conditions) or a whole molecule (a reagent) onto it and it moves with the arrow, as does a text typed right over or under it; drag within the row to reorder. In the panel you can put + or − before a molecule on an arrow (added, leaving). A double click on an arrow selects it with everything on it.

2.13 Side arcs on reaction arrows

A side arc shows something joining or leaving a reaction on the way, as $NAD^+ \longrightarrow$ NADH does.

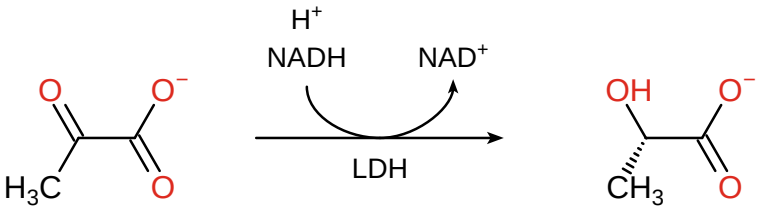


Fig. 10: Lactate dehydrogenase, with NADH coming in and NAD^+ leaving on side arcs

1. Choose the arrow tool. A small circle appears in the middle of each reaction arrow.
2. Drag out of the circle for an outgoing arc, or from the canvas to the circle for an incoming one, above or below the arrow.
3. Drag a text or a molecule onto the end of the arc. The arrow lengthens itself to fit, and shortens again if you take it away.

A further arc snaps to the length of the first; drag on to make it longer. To change an arc afterwards:

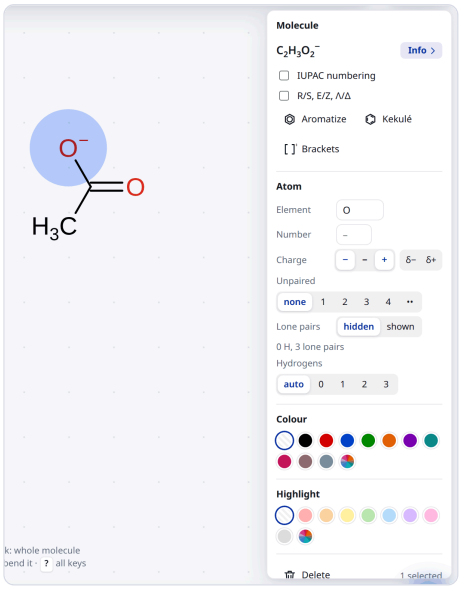
- drag its end to change its length, or across the arrow to move it, with its stack, to the other side,
- click it to select just the arc, and Del deletes it; what was at its end stays where it is, free,
- in the arrow's panel, Flip reverses the arrow and moves the arcs and stacks to the other side.

If you have set an arrow's length by dragging its end, the arcs leave that length alone, though Align reaction scheme does change it.

On an **equilibrium arrow** each of its two harpoons has its own arcs: an arc above it meets the upper harpoon and goes its way, an arc below meets the lower one and goes back. So the reduction of thioredoxin takes in 2 e^- and 2 H^+ above and gives them off below on the way back.

2.14 The panel on the right

The panel shows the properties of whatever is selected and lets you change them.



For a **whole molecule** it shows the formula (with the Info button, section 6.3), Carbons, IUPAC numbering, R/S, E/Z, Λ/Δ, Aromatize and Kekulé, Brackets, lone pairs, Draw the H, Colour and Highlight. For several molecules it adds Keep together.

For **one atom or part of a molecule**, an Atom section appears: Element, Number, Charge (− and + by one; also δ− and δ+), Unpaired electrons, Lone pairs and Hydrogens. Under the lone pairs it says how many the atom has.

For a **bond** it shows Order, Kind, Stereo and, for a double bond, 2nd line: Next moves the second line on, to the middle, one side or the other, and Auto gives it back to the program.

At the bottom there is always Delete and how many things are selected.

CHAPTER

3 Templates and structures from names

Templates in the bottom bar (or `Shift+T`) opens a collection of ready structures. On the left, under the search, are its groups: **Rings**, **Functional groups**, **Abbreviations**, **Compounds**, **Conformations and projections**, **Complexes**, **Amino acids**, **Sugars and nucleobases** and **Reagents and solvents**. The large ones are split further (**Rings** into aromatic, heteroaromatic, alicyclic and saturated heterocycles; **Conformations and projections** into chairs and boats, Newman, Haworth and Fischer projections): a group shows all of it under headings, a subgroup only its own. Next time it opens where you were last.

A click picks a template. A see-through preview then follows the pointer, and another click puts it down, as often as you like. `Esc` stops.

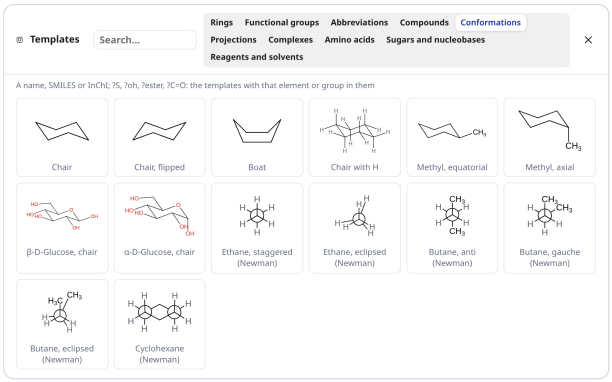


Fig. 12: Templates, chairs and Newman projections

3.1 Searching

Type part of a name into **Search...**, in English or Czech (`acid`, `glucose`, `chair`). An amino acid is also found by its code, which is on its card (`Phe` or `F`). When no template matches, the field works like **Name / SMILES** (section 3.5).

With a **question mark** in front, the search lists the templates that have a certain part in them, whatever they are called. Capitals do not matter.

- **a group:** `?oh`, `?Ts`, `?Boc`, `?Ph`,
- **a kind of compound:** `?ester`, `?amine`, `?ketone`, `?acid`,
- **an element:** `?S`, `?Cl`,
- **an amino acid by its three-letter code:** `?ala`,
- **any part, written as SMILES:** `?C=O`, `?C(=O)N`.

This is handy in teaching: `?ester` shows all the esters among the templates at once.

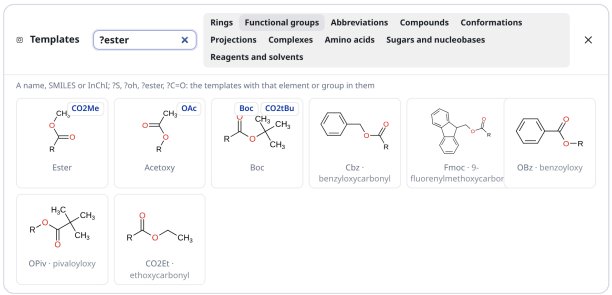


Fig. 13: Searching the templates with a question mark: `?ester`

3.2 Functional groups attach

The templates in Functional groups have a point of attachment. Pick a group and click an atom of your molecule: the group bonds to it, turned away from the atom's other bonds. Dragging from the atom aims the group. With Shift the atom becomes the group's first atom (COOH on pentane's end carbon gives pentanoic acid). A click on the empty canvas puts the group down on its own, on R.

A group with an abbreviation (Ph, Boc, OMe…) has a small button with that label on its card. It puts the group in as one atom with that label.

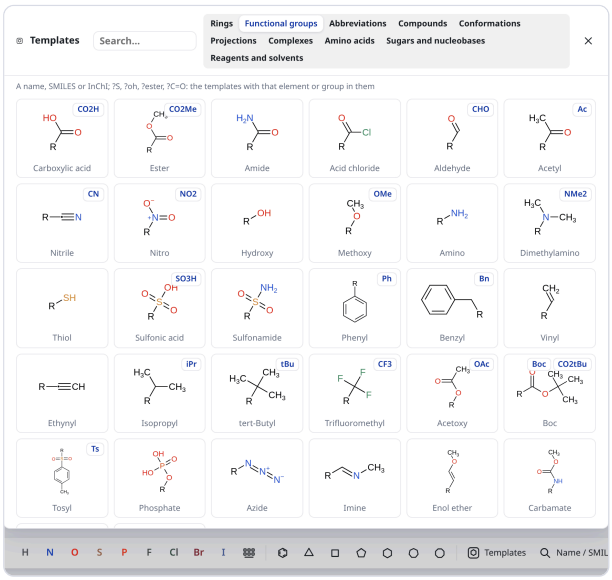


Fig. 14: Functional groups, with their abbreviations at the top right of the cards

3.3 Conformations and projections

- **Chairs and the boat** are drawn as in a textbook: parallel edges, axial bonds vertical, equatorial ones parallel to ring bonds. A chair is read as the molecule it shows, seen a little from above: its lower long edge in front, its upper one at the back, each group up or down as it points. So SMILES, InChI, Info and files get the stereoisomer in the picture (the β-D-glucose template is β-D-glucose, trans-1,2-dibromocyclohexane stays trans); other programs get it as wedges on the chair. A cyclohexene drawn in a chair's shape (the half-chair of an E2 product) is read the same way, though it can't be flipped or turned. Fused and bridged rings (decalins, steroids) get no stereochemistry from the picture yet.

  You can also draw a chair by hand with the bond tool: it is recognised by the shape every chair has, even if it isn't exactly the template's. Its opposite edges are parallel and two opposite corners point inwards (a zigzag). A regular hexagon, a Haworth ring and a boat don't have this shape. A ring with blunt tips, where you can't tell which chair it shows, isn't taken for a chair. When you point at a recognised chair or drag one of its atoms, the whole ring lights up in green-teal instead of the usual blue; the drawing itself doesn't change. Stereochemistry, Turn in 3D and the ring flip work on a recognised chair. Ring flip turns a chair into the other chair (section 5.5).
- **Newman projections** of ethane, butane and cyclohexane are molecules seen along a bond: the front carbon is the point in the middle, the back carbon the circle, and every group round them is an ordinary atom. Curved arrows, charges, lone pairs and R/S work on them as on any molecule: an E2 on cyclohexane, seen along C1–C2 and C5–C4 with the axial bonds straight up and down, is drawn with an arrow from the axial C–H to the bond seen end on (point between the middle and the circle) and one from C–Br to Br. A click right in the middle picks the front carbon, a click on the circle the back one. With a carbon of the projection selected, the Newman projection panel rewrites the groups (Front, Back: H, CH3, OH, Cl, Ph…), sets the Dihedral (0° eclipsed (syn), 60° gauche, 120° eclipsed, 180° anti) and turns the back carbon with Turn the back 60° in cyclohexane the ring groups stay and the back can't turn on its own. Files and SMILES get the stereoisomer the projection shows; molfile, CDXML and the other formats for other programs get it drawn plainly with wedges. Redraw makes an ordinary drawing of it, and drawings from older versions open as molecules.
- **Haworth and Fischer projections** (glucose, galactose, ribose, glyceraldehyde, alanine, serine…) carry stereochemistry, which is written to files as wedges.

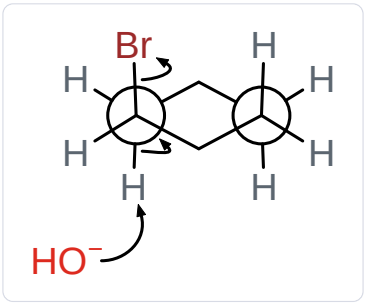


Fig. 15: An E2 on cyclohexane seen along C1–C2 and C5–C4: the Br and the H taken are trans-diaxial

3.4 Complexes

The Complexes group has the general shapes of coordination compounds: Linear, Trigonal planar, Tetrahedral, Square planar, Trigonal bipyramidal, Square pyramidal and Octahedral. A general atom M sits in the middle with ligands L round it, and wedges give depth. Replace M and L like any atom: click with an element from the bottom bar, press a key over the atom, or use the panel's Element field, where you can also type NH3, PPh3 or Cl.

A complex ion's charge belongs to an atom. The program counts bonds and lone pairs from the atoms' charges, and a charge written on brackets is just text. Take hexafluorosilicate, $[SiF_6]^{2-}$, as an example:

1. Put down an Octahedral complex, then change M to Si and all L to F (select them and type F into Element).
2. Select Si and set Charge in the panel to 2–, or press – twice over the atom. Si with six bonds is now fine and the red ring goes.
3. For the bracket notation, click the ion with the Brackets tool. Si already carries the charge, so do not write it on the brackets, or the picture shows it twice.
4. Add the K^+ ions and join the whole salt with Keep together (section 2.8).

There is another way, closer to the bonding picture: four plain Si–F bonds, and two fluorides F^- attached by coordination bonds / from F to Si. A dative bond does not count among Si's bonds, so Si stays neutral and the two F^- carry the charges.

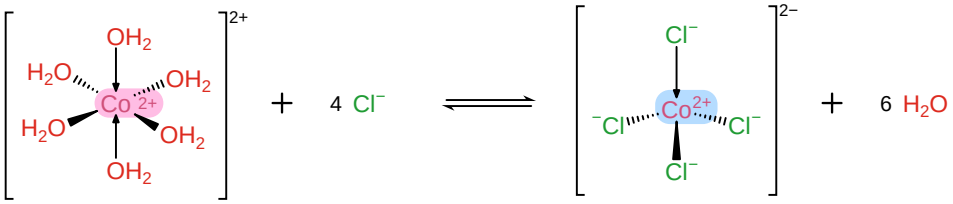


Fig. 16: Cobalt(II), octahedral (pink) and tetrahedral (blue): charges on the metal, brackets round each complex

To see any complex in space, use Turn in 3D (section 5.2), also a square planar one such as cisplatin drawn as a cross.

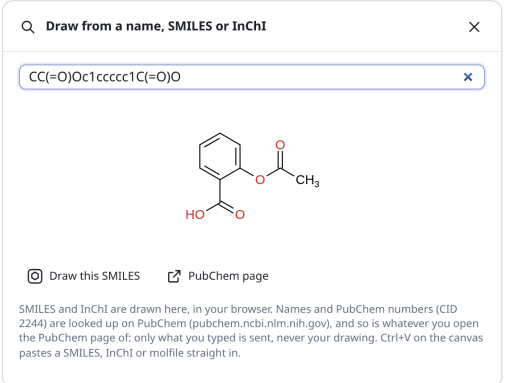
3.5 Structures from a name or SMILES

Click Name / SMILES in the bottom bar, or press /, and type:

- a **SMILES** (`CC(=O)Oc1ccccc1C(=O)O`) or an **InChI**, which is drawn as you type, on your own computer, even offline;
- a **name** (`aspirin`, `caffeine`) or a **PubChem number** (`CID 2244`), which is looked up in PubChem and needs the internet.

Press Enter and click where the molecule should go.

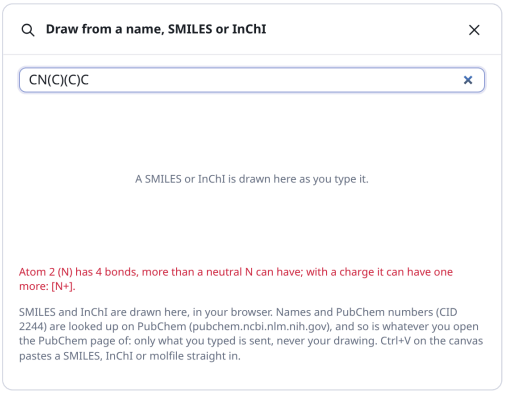
PubChem gets only what you typed, never your drawing. PubChem page opens the compound's page on PubChem.



When a SMILES has a mistake, the program says what and where, for example **Atom 2 (N) has 4 bonds, more than a neutral N can have; with a charge it can have one more: [N+].** When the mistake is a charge outside its brackets (N+ for [N+]), it offers the corrected SMILES: **Draw … instead**.

A SMILES or InChI copied from elsewhere can simply be pasted onto the canvas with `Ctrl+V` you do not need this window for that.

A halogen with more bonds is drawn as written: `Cl(=O)(=O)(=O)[O-]` as perchlorate with Cl=O double bonds (not Cl^{3+} with four O^{-}) and `Cl=O` as H–Cl=O. RDKit itself rejects such notation, so it gives no InChI or R/S for them.



CHAPTER

4 Mechanisms

In olomol, lone pairs and curved arrows are **part of the drawing**, not pictures laid on top. They belong to their atoms and bonds, so when you move, rotate or change a molecule they redraw themselves, even while you drag.

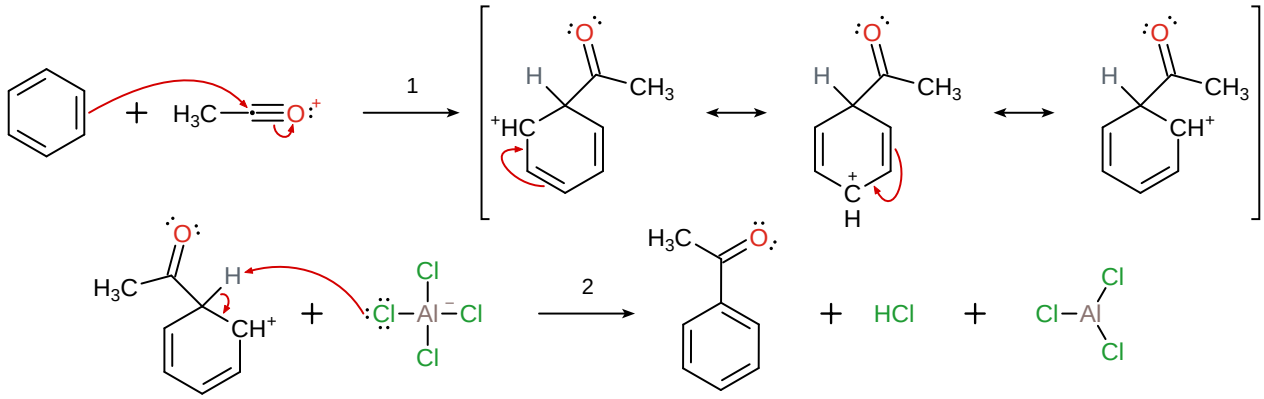


Fig. 19: Friedel–Crafts acylation of benzene in two steps, with the resonance structures of the σ-complex

4.1 Lone pairs and unpaired electrons

Choose lone pairs (ö: (:)) and click an atom, or drag a box over several atoms. If atoms are already selected, pressing the tool's button shows the pairs on all of them. In the panel the same thing is the Lone pairs switch: hidden / shown.

How many pairs an atom has follows from the chemistry: valence electrons minus charge, bonds, hydrogens and unpaired electrons. That is why the nitrogen of pyrrole has none and that of pyridine one. Add a charge or a bond and the count updates itself. Pairs are drawn as dots; Settings can switch them to bars (Bars (Lewis)).

4.2 Curved arrows and fishhooks

Choose the curved arrow (A) for an electron pair, or the fishhook among its variants (Shift+A) for one electron. Then:

1. Start where the **electrons come from**: a bond, an atom with a lone pair, or for a fishhook an atom with an unpaired electron (the fishhook starts at that electron).
2. Drag to where they **go**: an atom, a bond, or the dot of a new bond (see below), and release.

Instead of dragging, you can click the start and then the end. The tool stays on, so you can draw arrow after arrow. The program works out the path itself: it avoids labels, bonds, lone pairs and other arrows, and starts on the right side.

Arrows to a new bond. When the electrons make a new bond, the arrow can end between the two atoms, where the bond forms. While you drag a fishhook, or a curved arrow with Shift held (it can also be pressed in the middle of the drag), faint dashed lines lead from the electrons to every atom within five bond lengths that a new bond could go to, each with a dot in its middle. The lines in the pointer's direction are stronger. Drop the arrow on a dot and it ends at the new bond; drop it on an atom and it ends on the atom. This is how you draw hydrogen abstraction by a chlorine radical: a fishhook from Cl• and one from the H–C bond meet at the new Cl–H bond, and the other fishhook from the H–C bond goes to the carbon. Two radicals combining, or a nucleophile making a new bond, are drawn the same way.

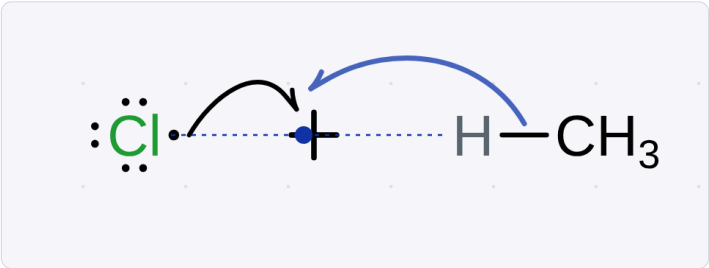


Fig. 20: A fishhook from the H–C bond dragged onto the dot of the new Cl–H bond, where the fishhook from Cl• already ends

It also checks the chemistry. It refuses an arrow from an atom that has no electrons to give and tells you why, for example This C has no lone pair or unpaired electron, so the electrons can't come from it. Start on a bond or another atom.

The colour of new arrows (red, say) is set in Settings → New arrows.

4.3 When an arrow does not look right

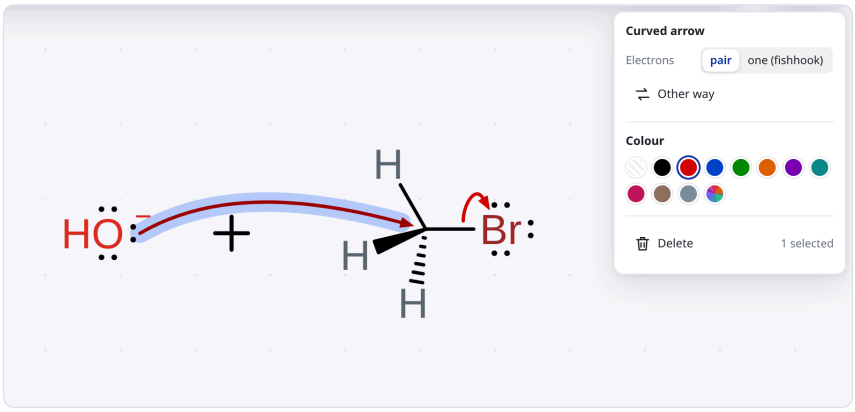


Fig. 21: A selected curved arrow and its panel

- **Drag** the arrow with the select tool to where it should run. The program picks the nearest good shape.
- Click Other way in the panel to draw the arrow the second best way, from the other side or from another lone pair. Click again for more; Best way returns the original shape.
- The Electrons switch turns the arrow into a fishhook and back (pair / one (fishhook)).

4.4 Orbitals

Orbitals are among the variants of the tool below the lone pairs: a p orbital, a hybrid orbital (a lone pair, σ*) and an s orbital the fourth variant, the overlap line, only draws dashed lines, dragged from one orbital to an orbital of another molecule. Click an atom to put one on it. A p orbital stands upright, a hybrid points away from the bonds, and dragging from the atom points it that way at once. Orbitals lie behind the bonds and labels, so the drawing stays readable.

- **Turning:** drag a lobe, with the orbital tool or the select tool. It turns in 15° steps and snaps to the bonds' directions, the perpendiculars to them and the lines between them; with Shift it turns freely. It turns, flips and is redrawn with its molecule.
- **Phase:** a click on a lobe with the orbital tool swaps the shaded and the white lobe; in the panel it is Other phase. The shaded lobe is grey and the other white. The paint tool colours the lobe you click; in the panel, the toggle above the colours, shaded or other phase, chooses which lobe they paint.
- **Size:** the lobes' size, for instance by the HOMO's and LUMO's coefficients, is set with − and + in the panel.
- **Overlap:** a lobe dragged onto an orbital of another molecule draws a dashed line between them. The two stay two molecules but are aligned together, like a diene and its dienophile. The line runs between the lobe you dragged and the lobe you dropped it on (a C–H bond's lobe and the lower lobe of a p orbital, say); dropped on the atom, it joins the lobes facing each other.
- **Arrows:** a curved arrow can start at a lobe or end on one, from a nucleophile's lone pair into the σ* of a C–Br bond, say.

On an atom with a label (O, N, Br) the lobes start outside the letters, and written hydrogens and the charge keep out of their way (NH beside the orbital, HO^- with its minus over the O). In Turn in 3D (section 5.2) the

p orbitals stand upright to the molecule's plane as you see it, on the side you drew them on. After Use this view they stay so, and a new p orbital on such an atom gets the same direction.

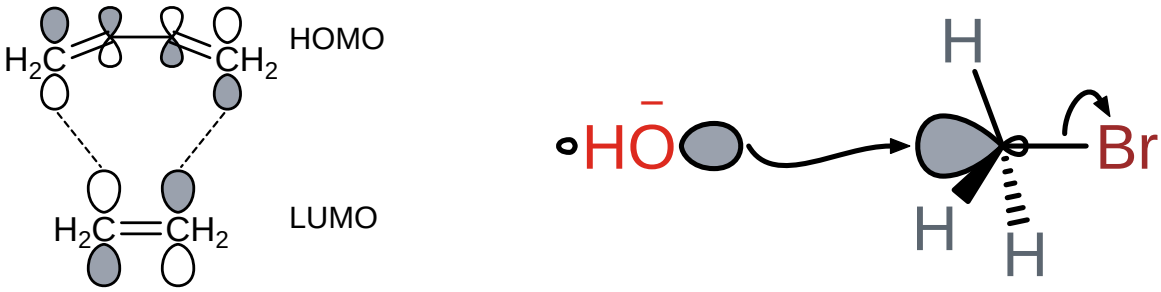


Fig. 22: Left, the diene's HOMO and the ethylene's LUMO in a Diels–Alder reaction: the lobes sized by the coefficients, dashed lines joining lobes of one phase. Right, an S_N2: the arrow from the hydroxide's lone pair into the σ* of the C–Br bond

4.5 Resonance structures, transition states and brackets

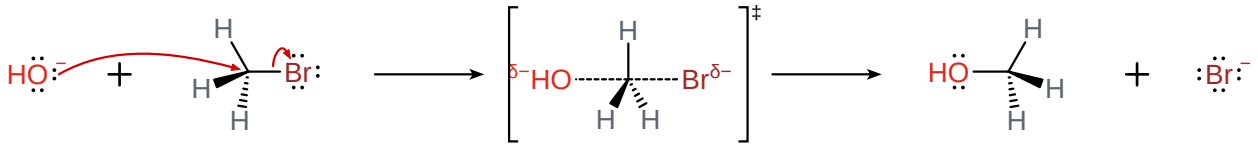


Fig. 23: S_N2: a transition state with partial bonds, partial charges and brackets with ‡

Resonance structures are separated by the resonance arrow ↔, a variant of the reaction arrow.

Brackets [ ] (K): drag a box, or click a molecule. The Brackets button in the panel puts them round the selected atoms. Brackets round a whole molecule suit a **transition state** or a **complex ion**, and the panel adds ‡, a charge or anything you type at the top right. Brackets round part of a chain mark a polymer's **repeating unit**: they cross the bonds leaving it and get n. Shape switches between square and round.

Transition states use the partial bonds and δ charges among the variants of the bond and charge tools. A δ+ or δ− that a curved arrow would cross moves to another side of its atom by itself. Redraw turns an S_N2 transition state sketched by hand into the textbook picture: both partial bonds in a line, and the other three bonds with wedges as you sketched them.

4.6 Aromatic rings

Aromatize in the panel draws a circle in aromatic rings, solid, or dashed if you choose that in Settings → Aromatic. Charged groups that look the same in all resonance structures (COO^-, NO_2, SO_3^-, guanidinium) are drawn delocalised with δ charges. With nothing selected, this applies to all molecules. Kekulé brings back single and double bonds.

Under the circle the single and double bonds remain, so the formula, lone pairs and files do not change, and other programs get an ordinary Kekulé structure. That is also why Kekulé brings back exactly the bonds that were there.

When you change a structure so that an aromatic ring or a delocalised group no longer makes sense (you delete a ring atom, or drag an acetate oxygen onto another atom), the program returns it to a Kekulé structure by itself.

5 CHAPTER Editing and arranging

5.1 Redraw

When a molecule looks muddled, perhaps after pasting a SMILES, select it and click **Redraw**. The program offers several drawings made by different methods, next to your **Current drawing**, and you click the one you like. `Ctrl+Z` undoes the choice.

The drawings are ranked. Those without crossing bonds or overlapping atoms, and with even bonds and angles, come first, and only the best few are shown. They are ranked once, when the quick methods are done; drawings from the slower ones (Indigo's clean-up, the 3D views) come a few seconds later and are added after them, so no drawing moves while you look. **Show all drawings** brings in the rest and **Show only the best** hides them again. A note under a drawing warns when bonds cross or atoms overlap in it.

Every drawing is checked: one that would change the molecule, its stereochemistry for example, is never offered. Redraw changes how a molecule looks, never what it is. Each drawing of a whole molecule is lined up with the page, turned by up to 15° so that most of its bonds lie at multiples of 30°, as a molecule pasted as SMILES is (a view of a 3D model keeps the view chosen for it).

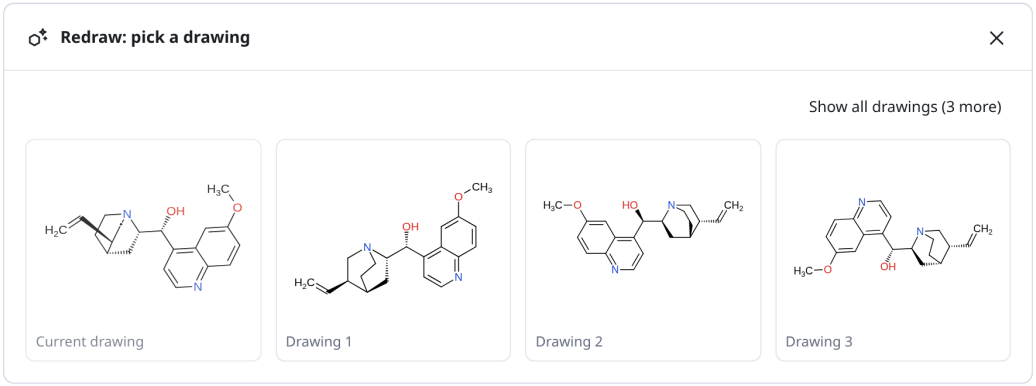


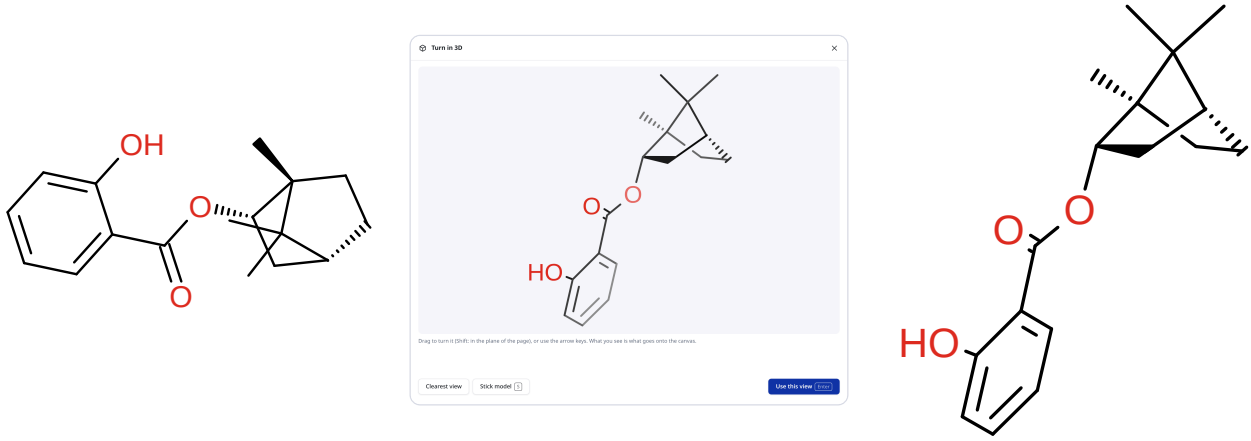
Fig. 24: Quinine: your current drawing, and the best of the drawings on offer

Drawings from a 3D model. Some drawings come from a 3D model of the molecule, turned and projected onto the page with wedges for depth. They are offered where they are the right picture: for cages and bridged rings (adamantane, norbornane, tropane), metal complexes, molecules with an expanded octet and S_N2 transition states. Any other molecule **Turn in 3D** shows in 3D. A large molecule such as taxol can take ten seconds or so, but the page does not freeze while you wait.

Molecules with one central atom with an expanded octet, or with five or more electron pairs round it (PCl_5, SF_6, SF_4, ClF_3, XeF_4, ClO_4^-, SO_4^{2-}), get their VSEPR shape, with room for the lone pairs. Sulfate is drawn as in a textbook, with the S=O double bonds in the plane of the page and O^- as a wedge and a hashed wedge. This part is still experimental (section 10.2).

5.2 Turn in 3D

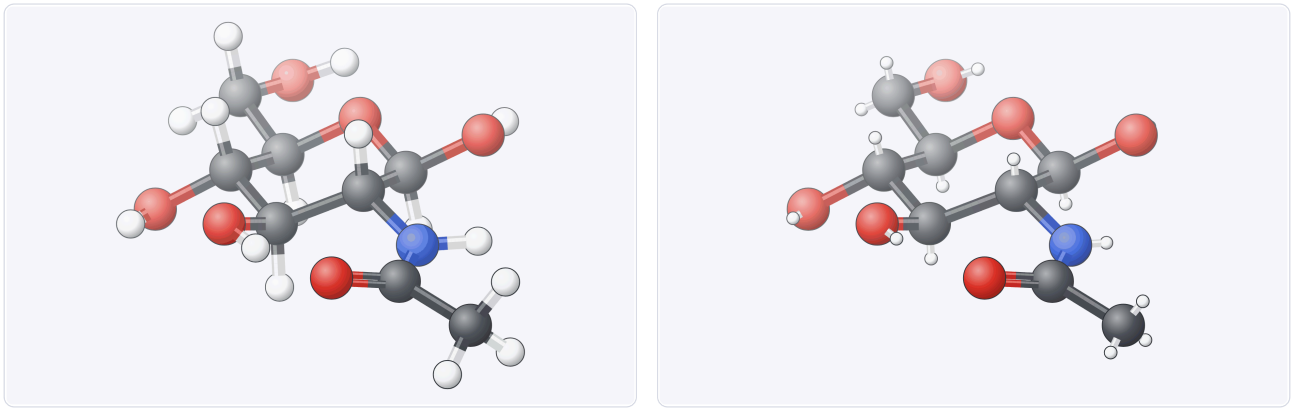
Sometimes a molecule reads best from one particular side. Select one molecule and click the cube next to **Redraw**. The program builds a 3D model, which takes a moment for a large molecule, and shows it just as it will be drawn, with the back paler so that you can see the depth.



as pasted | in the window, turned by hand | after Use this view

Fig. 25: Bornyl salicylate: as pasted, its bridge lies across the ring; turned by hand, the bornane looks as it does in a textbook

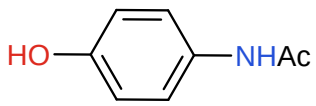
- **Drag** to turn it, or with `Shift` to turn it in the plane of the page.
- The **arrow keys** turn it in small steps, with `Shift` in the plane of the page.
- Clearest view goes back to the view the program found best, which is also where it starts.
- Stick model (`S`) shows the model itself instead of the drawing, turned the same way: its true bond lengths and angles, with every hydrogen. Groups written as shorthands are drawn out (see below). It has the drawing's colours and highlights of atoms and bonds too. Small hydrogens (`H`) draws the hydrogens the model adds small and close to their atoms, so that the skeleton stands out; those you drew as atoms stay as they are. It doesn't go onto the canvas: instead of Use this view there is Save picture (PNG, with SVG beside it), for notes next to the drawing, say, and `Esc` closes the window with your drawing as it was.
- Use this view puts the drawing on the canvas. `Ctrl+Z` undoes it. The paler back is only a help in this window; on the canvas you get an ordinary drawing.



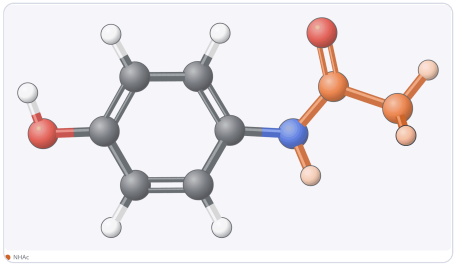
every hydrogen | `H`: small hydrogens

Fig. 26: The stick model of *N*-acetyl-β-D-glucosamine, turned as in its Haworth projection: every hydrogen, and with `H` the hydrogens small, so that the skeleton shows

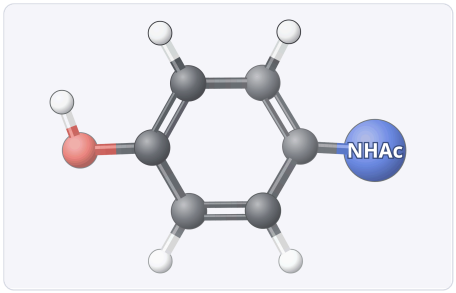
Groups written as shorthands (Ph, OMe, NHAc, OBz, also PPh_3 on a metal) are drawn out atom by atom in the stick model, so that the molecule's real shape shows. A group's carbons, hydrogens and bonds have a colour of their own, explained under the model. Oxygen, nitrogen and the other elements keep their usual colours, so you see at once what the group contains: the nitrogen and the carbonyl oxygen of NHAc, both oxygens of a benzoate (OBz). Draw out groups (`G`) is on to start with; switched off, it shows each group as one ball with its shorthand, for when the model with every atom is crowded. The window remembers both, `G` and `H`, until the tab is closed.



drawn with a shorthand



the group drawn out



G: the group as its shorthand

Fig. 27: Paracetamol drawn with the shorthand NHAc, and its stick model

The wedges are chosen so that R/S and E/Z stay as you drew them, and the 3D model itself is checked against your drawing. The model also has the drawing's conformation: a chair (from the templates, or drawn by hand and recognised) gives that chair (an axial OH stays axial, even where the other chair is more stable), cyclohexane in a Newman projection that chair, and a Newman projection of a chain the dihedral drawn, an eclipsed one too. A diene or an enone drawn s-cis (for a Diels–Alder) stays s-cis, though s-trans is more stable. If no such conformation can be found, the window says so and shows another. Sometimes a view cannot be drawn clearly: its wedges would not say the right R/S, or a bond points almost straight at you. The window then says so, and the button becomes **Use it anyway**: turn the molecule a little further, or use the view as it is.

Complexes work too. The whole complex is optimised by a force field (UFF), so each ligand keeps its proper shape, chelating ligands such as EDTA wrap round the metal and porphyrins stay flat, and where two bonds cross, the one behind is broken. If the program has no 3D model for a molecule, it tells you why.

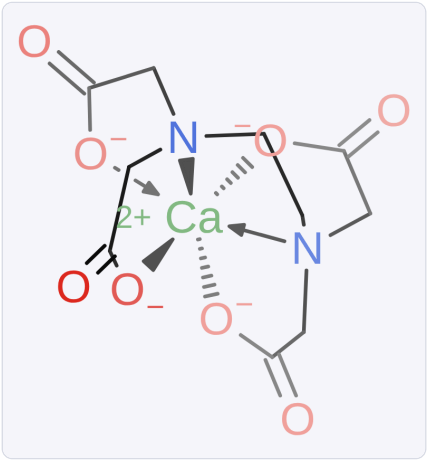


Fig. 28: EDTA round Ca^{2+}, built from a flat drawing

5.3 Redrawing only a part

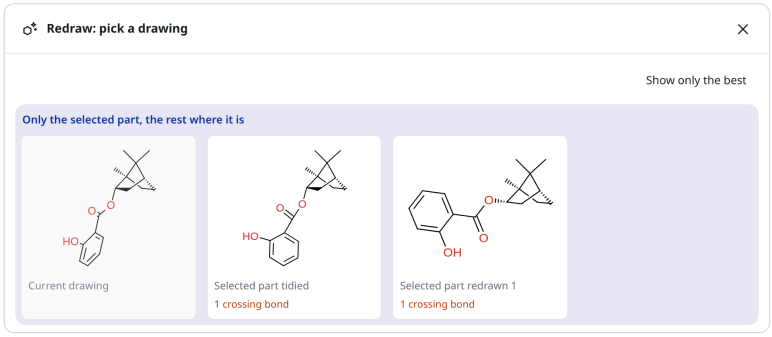
Often most of a molecule is just as you want it and only one part is a mess: a side chain, or a ring squeezed in. Select only that part, with a box, the lasso or Shift+click, and click **Redraw**.

The window then opens with a section of its own, **Only the selected part, the rest where it is**. In these drawings nothing outside your selection moves. Depending on the molecule you may see:

- **Selected part redrawn 1** (2, 3…) draws the part anew,
- **Selected part tidied** keeps its shape and cleans it up,
- **Selected part unchanged, reattached** keeps it exactly as drawn and sets it back in place, which helps after you have dragged a part away.

This is also how you get just one part of a molecule in 3D: turn the whole molecule (section 5.2), then clean up the part you want flat. Bornyl salicylate below was made that way. The bornane stays as it was turned, while the salicylate, its ring seen at a slant after the turn, is flat again.

Below, **Whole molecules** offers the usual drawings of the whole thing, should you prefer them. The example **Redrawing a part: the rest stays as drawn** in Help shows the difference on one molecule.



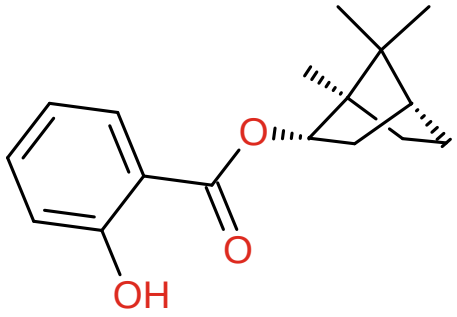


Fig. 29: Bornyl salicylate, turned in 3D (section 5.2), with only its salicylate selected: the window, and the drawing picked. The bornane has not moved

5.4 Align and grid

Select several molecules, and arrows and texts too if you like, and open **Align**:



- **Align reaction scheme** makes one row of the selected reaction: equal gaps, horizontal arrows, reagents going with their arrow, and texts under molecules on one line.
- **Align** lines up the left, right, top or bottom edges, or the middles.
- **Space evenly** works horizontally or vertically, with equal distances between middles or equal gaps.
- **Grid** arranges molecules in rows. Enter the number of **Columns** (or leave **auto**) and, if you wish, the **Gap** between cells in bond lengths (1.25 by default), and click **Arrange in a grid**. The grid stays where the selection was.

Molecules joined by a curved arrow move together. A text on an anchor always goes with its molecule, and free texts align on their own.

5.5 Flipping and straightening

- and in the top bar flip the selection, or with nothing selected the whole drawing. Wedges are swapped, so the molecule stays the same (R stays R).
- **Flip over a bond**: select part of a molecule, click the button, then click a bond. The selected part turns about the bond as an axis; with nothing selected, the smaller side does. The preview washes out what turns and shows in blue where it goes; Esc cancels. R/S is kept.
- **Ring flip** turns a chair into the other chair, axial ⇄ equatorial: click the button, then the chair (inside its ring or on one of its bonds). Each group stays on its face of the ring (up or down), so an axial group pointing up becomes an equatorial one pointing up, and cis and trans, R/S and D or L are kept: β-D-glucose, all equatorial, becomes the all-axial chair and is still β-D-glucose. Every ring atom stays where it was (left, right, back or front), so the class sees the same carbon go from axial to equatorial; a group such as CH_2OH or phenyl turns as a whole. The preview shows the other chair in blue. The flip is animated through a boat (one tip drops, then the other rises); **Settings** → **Animations** turns that off. Shift+click puts the other chair beside the first, with an equilibrium arrow between them: the picture for a handout. Another click flips the chair back; Esc ends.

  A chair from the templates (**Templates** → **Conformations and projections**, turned, enlarged, mirrored or with groups added) flips, and so does one drawn by hand if it is recognised (it turns green-teal under the pointer). The flipped chair is drawn in the template's shape. A flat six-membered ring, a hexagon or a Haworth projection, becomes a chair: pointed at, it turns green-teal with the chair see-through over it, and a click draws it. Each group goes axial or equatorial by its face, from its wedge or hashed wedge (a Haworth's group up or down), so the molecule stays the same. It is always the templates' chair, its left tip raised (a sugar $^4C_1$, β-D-glucose all equatorial); the ring flip gives the other one. A group whose side the drawing doesn't say goes equatorial, with a wavy bond where it sits on a stereocentre. A ring with a double bond (a cyclohexene) and fused or bridged rings (decalins, steroids) are refused with a message.

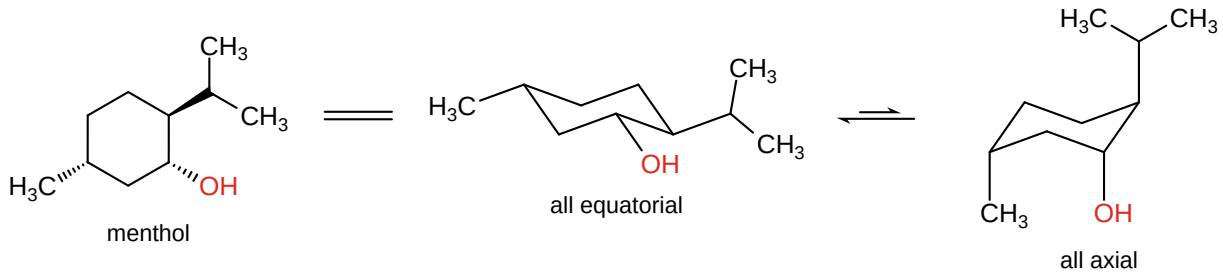


Fig. 31: Menthol drawn as a flat ring with wedges = its chair, every group equatorial; the ring flip gives the other chair, every group axial, and the equilibrium favours the first

Cyclohexane in the template's Newman projection (seen along C1–C2 and C5–C4) flips too: both projections stay where they are, C3 and C6 change sides, and each group on the four carbons seen end on goes into the other slot on its face of the ring, axial ⇄ equatorial. Trans-diaxial Br and Cl become diequatorial, and in 3D go from anti to gauche. Groups on C3 or C6 stop the flip.

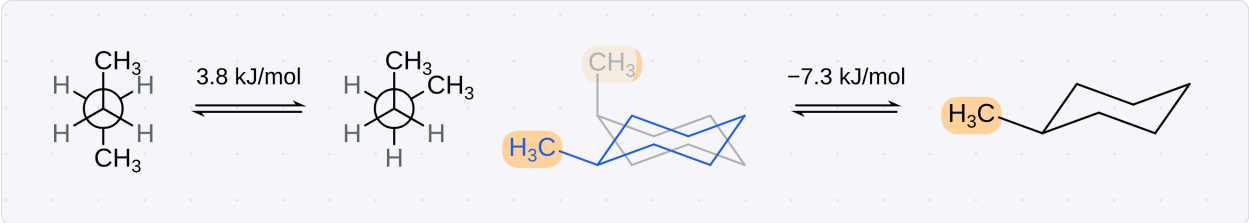


Fig. 32: Ring flip: the other chair under the pointer, see-through in blue; a click draws it

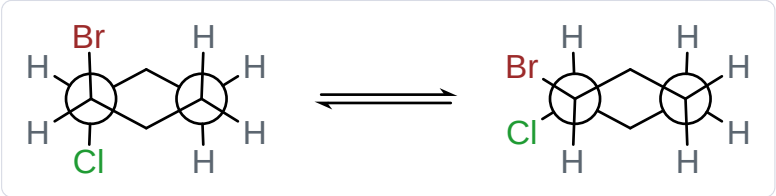


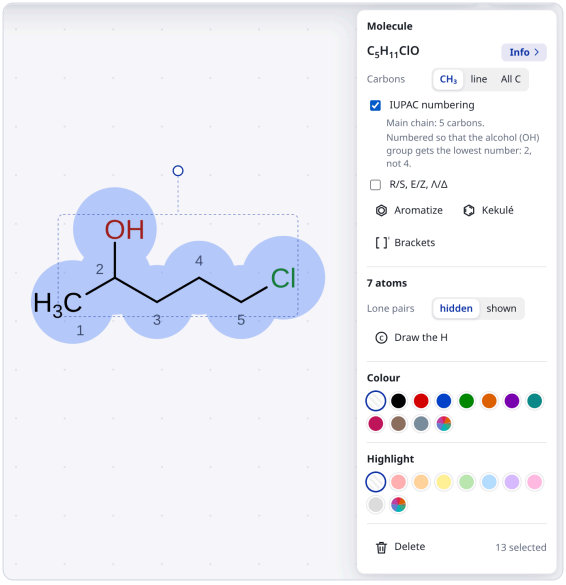
Fig. 33: Cyclohexane in a Newman projection flipped, with Shift+click beside the first: the trans-diaxial Br and Cl are now diequatorial

- **Turn a chair** turns a chair a third of the way round its axis, anticlockwise (with Shift clockwise): each ring atom moves two corners on with its groups, which stay axial or equatorial, up or down. It is the same molecule in the same conformation, only seen turned; three turns bring it back. When a flat ring becomes a chair with its atoms on other corners than you wanted, turn it until they are where you want them; the ring flip gives the other conformation.
- **Horizontal / vertical** makes a bond straight. Click the button, then the bond: the selection turns if the bond is in it, otherwise the whole molecule. Another click on the bond turns it a quarter further. With one bond selected, its molecule turns as soon as you press the button.

6 CHAPTER Atom numbering and the Info card

6.1 IUPAC numbering

Select a molecule and tick **IUPAC numbering** in the panel. The parent chain or ring is numbered by the IUPAC rules (2013 recommendations), and the numbers are worked out again after every change: add Cl to the other end of hexane and C1 moves there. The panel says which rule decided, for example **Numbered so that the alcohol (OH) group gets the lowest number: 2, not 4.**



The program knows how to choose the parent chain or ring: by the senior principal group (acid > ester > acyl halide > amide > nitrile > aldehyde > ketone > alcohol > thiol > amine), a ring before a chain, then the longest chain with the most multiple bonds and substituents.

It gives the lowest locants to ring heteroatoms, the principal group, multiple bonds (double before triple) and substituents, and finally goes by alphabetical order. Only the parent is numbered, as in a name.

6.2 Your own numbers

Fused, bridged and spiro rings (naphthalene, steroids) have numberings of their own that the program does not work out. For them, and for assigning NMR signals, use the atom number tool, a variant of the text tool. Click atoms in the order you want them numbered; clicking again removes a number.

To change one atom's number, use the panel's **Number** field. **Remove own numbers** deletes them all. Numbers are kept in KET files, links and pictures.

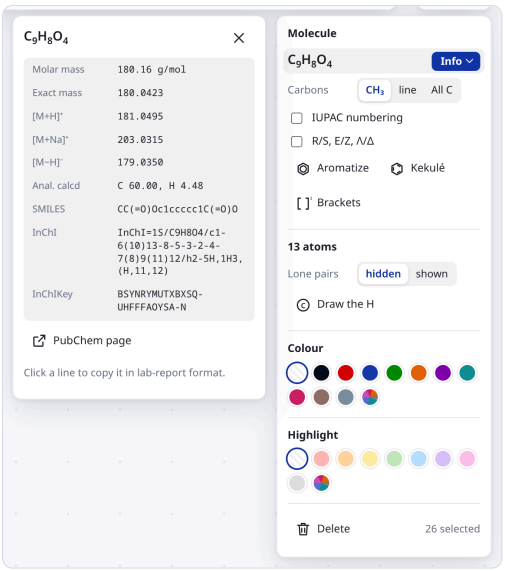
6.3 The Info card

Select a molecule and click **Info** next to the formula in the panel. A card opens beside the panel with the numbers a lab report or experimental section needs:

- **Molar mass** and **Exact mass**,
- ions for HRMS: $[M+H]^+$, $[M+Na]^+$ and $[M-H]^-$ (for an ion, $[M]^+$),
- **Anal. calcd** for C, H, N and S,
- SMILES, InChI and InChIKey.

Click a row to copy it. You get only the formula, ion and number, with no words, so it fits a report in any language: for example `C9H8O4 [M+H]+ 181.0495` or `C9H8O4: C 60.00, H 4.48`. Then paste it into your text.

Everything on the card is computed on your computer. The card closes when you select another molecule or click the empty canvas.



6.4 Finding a compound on PubChem

PubChem page on the Info card opens the compound's page on PubChem. It is the only thing on the card that sends anything out: the molecule's InChIKey, by which PubChem finds the compound, and its SMILES too if PubChem has no exact match.

What you draw is not always exactly what PubChem has. You may have left a stereocentre undefined, or drawn an isotope. Then, instead of guessing, olomol shows a page of cards with PubChem's picture, name and number for each candidate. Click a card to go to that compound. The heading says how they differ:

- **Your drawing leaves stereochemistry open**: PubChem has it just as you drew it (the first card, marked **as drawn**), and the others define more of it, in agreement with what you drew. One of those is often what you meant.
- **Not with exactly this stereochemistry**: nothing matches exactly, but these agree with the stereocentres you did draw.
- **This stereoisomer isn't on PubChem**: these have the same atoms and bonds, with other stereochemistry.
- **Not with exactly these isotopes**: these have the same atoms and bonds, with other isotopes or none.

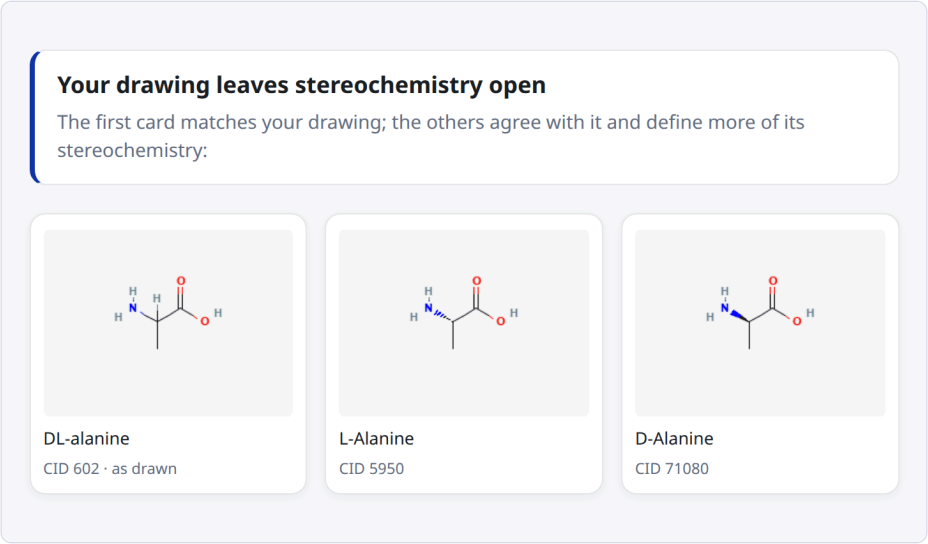


Fig. 36: Alanine drawn without stereochemistry: PubChem has DL-alanine, and also L- and D-alanine

If PubChem has nothing at all, the page says so and offers **Search PubChem**.

7 CHAPTER Colours and highlighting

7.1 Colour

Colour changes lines and letters. Select atoms, bonds, arrows or text and click a colour under Colour in the panel; the crossed-out circle is Default colour. Or use the tool ● at the bottom left, with ten colours among its variants, and click or box what you want to colour.

The rainbow circle after the colours (More colours, or a colour code) opens a larger choice: a row Used last, a grid Colours and a field for a colour code (`#cc0055`, `#c05`, `rgb(204, 0, 85)` or a name like `teal`; Enter uses it). The circle next to the field opens the system's colour picker. The program remembers the colours you use and offers them among the tool's and panel's colours too.

When Atom colours in Settings is set to Black, the elements are drawn in black but your own colours stay, so red arrows on black structures stay red.

7.2 Highlighting and filled rings

Highlighting is a soft coloured background behind atoms and bonds, as RDKit draws it. It marks a group, a reaction centre or the common part of several molecules.

Use the highlighter at the very bottom left, with eight colours. Click atoms and bonds or box them; a second click takes the highlight off. The panel does the same under Highlight, and here too the rainbow circle offers more light colours.

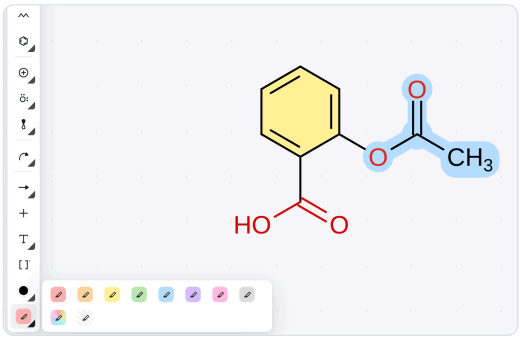


Fig. 37: A filled ring, a highlighted ester and the acid in red

A click inside a ring fills it with colour. Round written atoms (O, N, CH_2) a round cut-out remains, so the colour does not cover the letters.

With the select tool, a click into a filled ring selects the ring, a double click the whole molecule, and dragging moves it. A smaller highlight always lies over a larger one (the orange difference over the blue common part).

A fill goes when you break the ring by deleting a ring atom or bond. Otherwise you can remove it with the highlighter's No highlight variant (click inside the ring), with the eraser (click inside the ring), or with No highlight in the panel when all the ring's atoms are selected.

7.3 Example: what molecules have in common

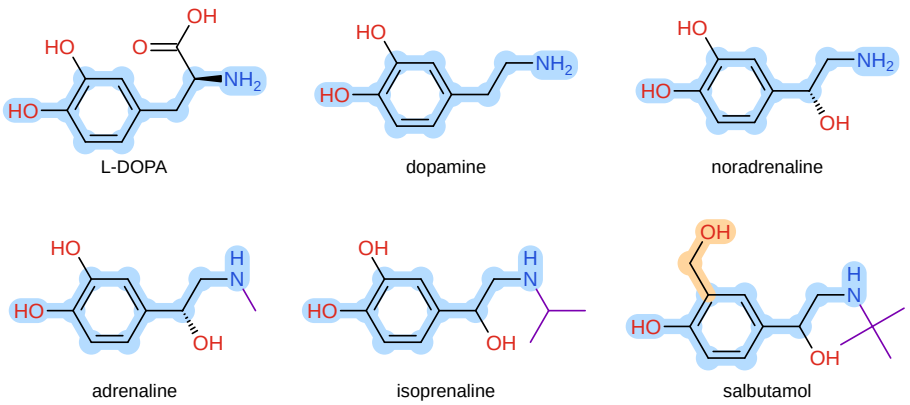


Fig. 38: Catecholamines and related drugs: the common part in blue, salbutamol's main difference in orange, the groups on nitrogen in purple

L-DOPA, dopamine, noradrenaline and adrenaline are made in the body one from another; isoprenaline and salbutamol are drugs. The common part, a phenol with a C–C–N chain, is **highlighted in blue** and turned the same way in every molecule. Salbutamol, an asthma drug, has its main difference **highlighted**

in orange: CH_2OH in place of one OH, so the enzyme COMT does not break it down and it acts for hours, not minutes. The groups on nitrogen are **painted purple** with the paint tool: the bigger the group, the more the compound acts on β-receptors.

To make a picture like this:

1. Draw the first molecule, copy it (`Ctrl+C`, `Ctrl+V`) and edit the copy. The common part stays turned the same way everywhere, which molecules pasted from SMILES would not do.
2. Select everything, enter 3 **Columns** in **Align** and click **Arrange in a grid**.
3. Select the common part (drag a box, `Shift`+click) and click the blue **Highlight** in the panel. Do the same with orange for the difference.
4. Colour the groups on nitrogen with the ● tool or with **Colour** in the panel.

8 CHAPTER Files, export and links

The way out of olomol depends on what you want to do next:

You want to…	Use
keep working on a drawing later	**Save** (`Ctrl+S`): a KET file, with everything in it
put it into Word, PowerPoint or Google Docs	**Copy as picture** (`Ctrl+Shift+C`), then `Ctrl+V` there
print it, or go on editing it in Inkscape	**SVG**
send it to a colleague or students	**Copy link**, or the KET file
open it in ChemDraw or another chemistry program	**Structure file**: Molfile, SDF, SMILES or InChI
start a calculation from it	**Structure file**: XYZ

8.1 Save and open

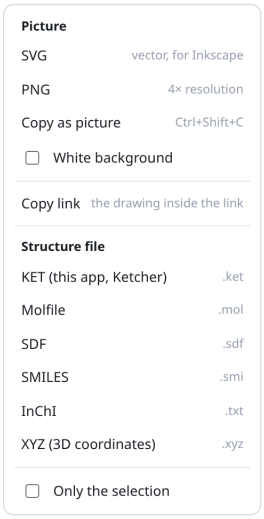
Save (`Ctrl+S`) stores the drawing as a **KET** file. It opens here again with everything in it: lone pairs, curved arrows, colours, highlights and numbers. Ketcher opens it too, showing lone pairs and arrows as pictures. For your own work, KET is the best choice.

When saving, the program asks for a file name. Chrome and Edge also let you choose the folder; in Firefox, a **Save as** window asks for the name and the file goes where downloads go.

Open (`Ctrl+O`) reads KET, molfile, SDF, SMILES, RXN, CDXML and CDX (ChemDraw), CML and XYZ. A drawing (KET, a reaction, CDXML) opens in place of the one you have. A file of molecules only (molfile, SDF, SMILES, XYZ) goes into the drawing you have, like a template: click where it should go. An XYZ file from a quantum chemistry program has no bonds, so the program adds them from the distances between atoms, works out bond orders and stereochemistry, and draws the molecule in 2D.

8.2 Exporting pictures and files

The **Export** menu in the top bar offers:



- **SVG** (**vector, for Inkscape**): a clean vector picture in which text stays text. It is the best choice for print, posters and further editing.
- **PNG** (**4× resolution**): a raster picture with a transparent background, or a white one if you tick **White background**.
- **Copy as picture** (`Ctrl+Shift+C`): a PNG on the clipboard, transparent or with **White background**.
- **Copy link**: see section 8.4.
- **Structure file**: KET, Molfile, SDF, SMILES, InChI and XYZ (3D coordinates).

With something selected, **Only the selection** is ticked and only the selection is exported. Untick it to export the whole drawing.

Structure files carry atoms, positions, charges, isotopes, radicals and wedges in standard formats. Reading them back has been tested in olomol, RDKit and Indigo, not in other programs. **Lone pairs, curved arrows, brackets, partial bonds and colours are kept only in KET and in pictures.**

An **XYZ** file holds 3D coordinates with all hydrogens. It is a starting geometry for calculations (Gaussian, ORCA and the like), optimised by a force field only, not by quantum chemistry. A metal complex is built as in **Turn in 3D**, optimised as a whole by the universal force field (UFF) on its coordination polyhedron; UFF makes metal–ligand bonds somewhat shorter than they are (Zn–N in ZnTPP 1.95 Å instead of 2.04 Å). A complex **Turn in 3D** can't build (ferrocene) isn't written, and the program says why. The coordinates are worked out in the background: a panel shows that it is working while you keep drawing, and **Save XYZ file** saves them when they are ready, for the drawing as it was when you asked. The suggested file name is the molecule's InChIKey, so several structures from one drawing don't overwrite each other. Check the warning about stereocentres with no R/S drawn: the file then holds just one of the possible stereoisomers.

8.3 Into Word, PowerPoint and Google Docs

Select what you want to take over, or nothing for the whole drawing. Press `Ctrl+Shift+C`, or choose **Export** → **Copy as picture**, and then `Ctrl+V` in Word, PowerPoint or Google Docs.

SVG is the sharpest in print: Word and PowerPoint insert it (Insert → Pictures) and it does not blur when enlarged. For ACS journals, set the style in **Settings** to **ACS 1996** (bonds 14.4 pt, lines 0.6 pt, Arial 10 pt).

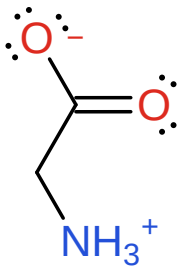
8.4 Links

Export → **Copy link** makes a link that **holds the whole drawing**, after the # sign, which the browser does not send to the server. Whoever opens it sees your drawing, and their own comes back with `Ctrl+Z`. Some chat programs cut long links short; if that happens, send the KET file.

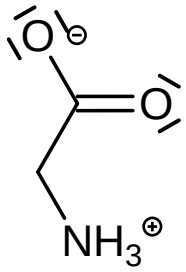
9 CHAPTER Settings and keyboard shortcuts

9.1 The look of the drawing, language and window

The look changes most with how **charges**, **lone pairs** and **atom colours** are drawn. On the right is the same glycine in the default look, and with circled charges, lone pairs as bars (Lewis) and black atoms. Settings apply to the whole drawing and to exported pictures.



default



⊕ ⊖, bars, black

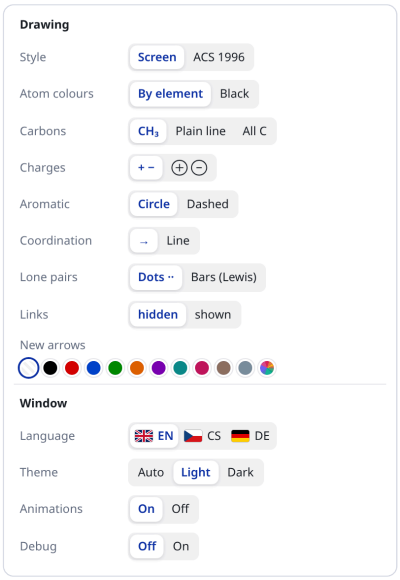
Settings (⚙ at the top right):

Drawing

- Style: Screen, or ACS 1996 (ChemDraw's style for ACS journals; pictures then come out at that size).
- Atom colours: By element, or Black (your own colours stay).
- Carbons: CH_3, Plain line, or All C for new drawings.
- Charges: + −, or circled ⊕ ⊖.
- Aromatic: Circle, or Dashed (the circle dashed).
- Coordination: → (an arrow from the donor), or Line (plain lines, as complexes are often drawn); with depth they are wedges either way.
- Lone pairs: Dots ··, or Bars (Lewis).
- Links: hidden, or shown (the invisible links of Keep together groups, on screen only).
- New arrows: the colour of new curved arrows.

Window

- Language: flag buttons EN, CS, DE. Without a choice the browser's language is used, or English if the program does not have it. The page reloads, and the drawing with its zoom and position stays. Templates can be searched in English or Czech; PubChem knows English names only. The end of the address, `?lang=en`, `?lang=cs` or `?lang=de`, chooses the language too.
- Theme: Auto (as the system), Light, or Dark.
- Animations: On or Off, short animations such as the ring flip. Until you choose, they follow the system: off when it asks for less motion.
- Debug: debug mode shows how the program decided (layout methods, label boxes, arrow candidates). It is meant for developers, but when you report a drawing problem, a screenshot with it on can help.



9.2 Keyboard shortcuts

The ? key or Keyboard shortcuts in Help (section 1.4) shows them too. Letters and digits do different things depending on what is under the pointer: an atom, a bond, or empty space.

Over an atom

C N O S P F H I	changes the element
L B	Cl, Br
+ −	charge
.	unpaired electron (again: two side by side, then none)
:	lone pairs on/off
Del	deletes it

Over a bond

1 2 3	single, double, triple
1 again	wedge, hashed wedge, both from the other end, plain
Shift+1	the same, backwards
D	dative bond, again hydrogen bond, again partial bond
Del	deletes the bond

In Turn in 3D

Arrow keys	turn it (Shift: in the plane of the page)
S	stick model, and back
G	in the stick model: draw out groups
H	in the stick model: small hydrogens
Enter	Use this view
Esc	close the window

Writing text

Enter Esc	finish
Shift+Enter	new line
Ctrl+, Ctrl+.	subscript, superscript
Ctrl+B Ctrl+I	bold, italic

Tools (pointer over empty space)

V	select
E	eraser
N	draw with nitrogen (likewise O, S, P, F, H, I, L = Cl, B = Br; C: carbon again)
1	single bond (again: wedge, again: hashed wedge)
2	double bond
3	triple bond
Z	chain (zigzag)
R	benzene (again: the next ring, 3- to 8-membered)
5	5-membered ring
6	6-membered ring
+	positive charge
−	negative charge
.	unpaired electron
:	lone pairs
A	curved arrow (electron pair)
Shift+A	fishhook (one electron)
Shift+T	Templates
X	reaction arrow
T	text
K	brackets
D	dative bond, again hydrogen bond, again partial bond

Other keyboard layouts Digits work by the key's position, in the top row of e.g. a Czech keyboard too. + over an atom raises its charge there as well; choose the positive charge tool with + on the number pad.

Anywhere

Esc	cancel; again: the Select tool; again: nothing selected; again: box or lasso
Ctrl+Z Ctrl+Shift+Z Ctrl+Y	undo, redo
Ctrl+C Ctrl+X Ctrl+V	copy, cut, paste (SMILES and molfile too)
Ctrl+Shift+C	copy as picture (PNG), for Word, PowerPoint, Docs
Ctrl+A	select all
Del	delete the selection
Arrow keys	move the selection (Shift: further)
Ctrl+S Ctrl+O	save, open
Ctrl+wheel	zoom
space+drag	move the canvas
/	draw from a name, SMILES or InChI
?	this overview

CHAPTER

10 Installing, limitations and reporting problems

10.1 Installing as an app and working offline



After the first visit olomol works **without the internet** too, because the browser keeps all its files. Offline, only the PubChem look-ups do not work.

Installed as an app, it has its own window and an icon on the desktop or in the Start menu, and it opens at once:

- **Chrome and Edge:** use the button at the top right (the first icon in the picture) or the install icon in the address bar.
- **Firefox on Linux** cannot install it as an app, but the program works normally in a browser window there, offline too.

10.2 Known limitations

olomol is a testing version. This is what it cannot do yet, or can do only in part:

- **Firefox on Linux** cannot install the program as an app. Use Chrome or Edge, or work in a browser window.
- **Drawings of metal complexes and molecules with an expanded octet** made from a 3D model in Redraw are experimental: they sometimes look odd or are not offered at all. The XYZ export is only a starting geometry, optimised by a force field.
- **A name from a structure** is something the program cannot make. The other way round, a structure from a name goes through PubChem, so it needs the internet and English names.
- **IUPAC numbering** handles the parent chain and simple rings. Fused, bridged and spiro rings must be numbered by hand with the atom number tool .
- **Lone pairs, curved arrows, brackets, special bonds and colours** are carried only by KET, links and pictures, not by molfile or SMILES.
- **Chairs** give stereochemistry only on their own, not fused or bridged; boats give none. Ring flip and Turn a chair refuse fused and bridged rings and rings with a double bond.
- **Copying pictures to the clipboard** is not allowed by some browsers. The program tells you so; export a PNG instead.
- **The drawing in the browser** lives only in this browser on this computer and does not sync between computers. To carry it over, use KET files or links.

10.3 Problems and ideas

Every message is welcome, even about a small thing. Click the bug at the top right (or Report a problem or an idea in Help). A window opens with a table of what helps to find a fault: the program's version, the browser, the system, the window size and, if you leave With the drawing (a link that holds it whole, so I can see what you saw) ticked, a link to the drawing.

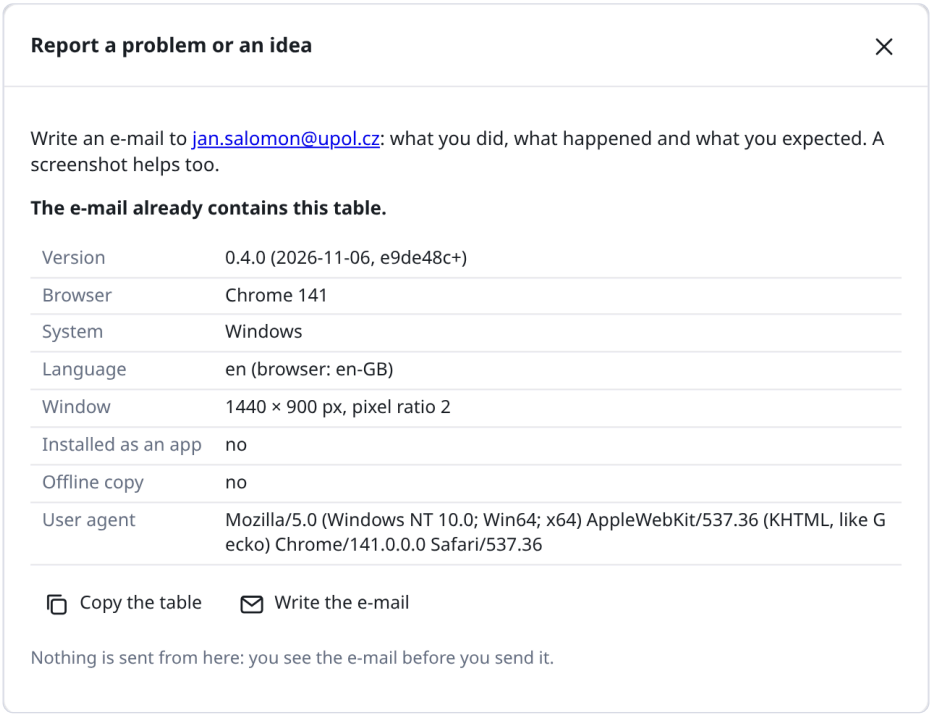


Fig. 42: The window for reporting a problem

1. Click **Write the e-mail**. A new e-mail to jan.salomon@upol.cz opens with a few questions that are enough to answer: what you did (briefly is fine), what happened and what you expected. The table is already in it.
2. A link to a drawing is too long for an e-mail, so with the drawing, click **Copy the table** and paste the table (`Ctrl+V`) at the end of the e-mail.
3. A screenshot or a KET file helps too.

Nothing is sent from here: you see the e-mail and send it yourself. If no e-mail opens after the click (you use webmail only, say), write to the address by hand and paste the table all the same. The program's version is also at the bottom left and in **About**.

APPENDIX

A How olomol is built

This appendix is for those who want to know what is under the bonnet: computing teachers, school network administrators, developers and curious chemists. You do not need it to use the program.

A.1 The big picture

olomol is a **static web page**: HTML, JavaScript and WebAssembly, nothing more. It needs no application server, database or accounts. Any web space with https (a school server, GitHub Pages) is enough, and everything else runs in the user's browser. Its own code is about 24,000 lines of JavaScript.

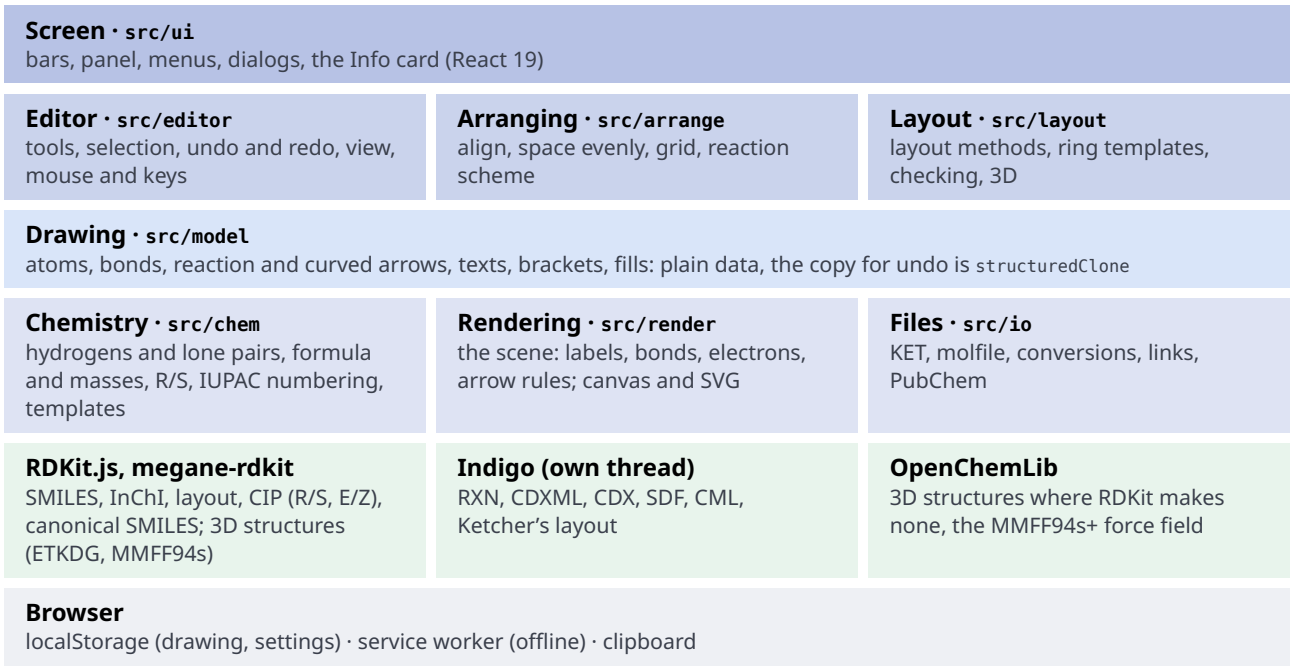


Fig. 43: The program's layers. The top three rows are its own code (folders in `src/`); the green row are WebAssembly libraries, downloaded only when first needed.

A.2 What each part does

Folder	What is in it
`src/model`	The drawing as data. Coordinates are in bond lengths, the y axis points down as on screen. `graph.js`: molecules (connected parts), smallest rings.
`src/chem`	Chemistry computed by its own code: hydrogens and lone pairs (`valence.js`), formula and masses, R/S labels, IUPAC numbering (`numbering.js`), templates, chairs and projections, delocalised groups (COO^-, NO_2).
`src/render`	After every change the **scene** is computed once: where labels go, how bonds look, where lone pairs sit and which way curved arrows run. The canvas, the SVG export and finding what is under the pointer all use it. The pictures in this manual are exports of that same scene.
`src/editor`	The editor and tools: selection, dragging, bonds, rings, templates, history (200 steps), keys.
`src/arrange`, `src/layout`	Aligning and new layouts: several methods (RDKit, CoordGen, Indigo, RDKit's ring system templates, 3D from RDKit or OpenChemLib, metal complexes by UFF), each drawing of a whole molecule turned onto the 30° grid.
`src/io`	Files: KET (reading and writing), molfile V2000/V3000, conversions through RDKit and Indigo, XYZ, links, PubChem.
`src/ui`	The screen in React: bars, panel, menus, dialogs, the Info card.

Folder	What is in it
`src/i18n`	Languages. The key is the English text, `cs.js` and `de.js` are translation tables; a test reports missing texts.

A.3 Rules that are not from the libraries

- **Lone pairs** are counted as valence electrons − charge − bonds − hydrogens − unpaired electrons. Tests check that the counts match RDKit's.
- **Curved arrows** are not drawn by hand: for each arrow the program makes hundreds of candidate Bézier curves and gives each a "cost". It pays for crossing a label, bond, lone pair, ring interior or another arrow, for a bend that does not suit the arrow's length (short ones bend more, long ones less), for a lopsided arc and, for a new bond, for a head that does not come from the electrons' side. The cheapest wins; Other way picks the next one that looks different. Debug mode (Settings → Debug) shows the candidates with their cost.
- **A new layout** never changes the molecule: each drawing is turned into a canonical SMILES with stereochemistry and compared with the original. Any that differs is dropped.
- **IUPAC numbering** follows the IUPAC 2013 recommendations (parent chain or ring, lowest locants, alphabetical order) and stores the reason with the numbers, which the panel shows.
- **Flipping** swaps wedges and hashed wedges, so the mirror image stays the same molecule; tests check that too.

A.4 Data and files

- **Its own format** is KET, the JSON of Ketcher. Molecules, arrows, "+" and texts are written in the standard way, so Ketcher and the Indigo library open the file. Lone pairs and curved arrows are in it also as pictures (so that Ketcher shows them), and an `olomol` section in the file's root carries what only olomol uses: colours, highlights, ring fills, arrows anchored to atoms and bonds. Other programs skip it.
- **Saving as you go:** the drawing (as KET) and the settings are in the browser's `localStorage`.
- **A link to a drawing:** KET, compressed (`deflate-raw`) and written in base64url after `#d=`. The browser does not send the part of an address after # to the server, so a drawing in a link never passes through the server olomol is on.

A.5 What leaves the computer

When	What, and where to
Looking up a name or CID	only the typed text, to PubChem PUG REST (`pubchem.ncbi.nlm.nih.gov`)
PubChem page	the molecule's InChIKey (or the typed SMILES or InChI), to PubChem; if PubChem has no exact match, its SMILES too
Loading the page	an ordinary request to the server olomol is on; libraries, fonts and icons are part of the page, nothing is fetched from elsewhere
Anything else	nothing: no analytics, no cookies, no accounts

A.6 Offline and installing

The build (`npm run build`) makes a **service worker** (`scripts/pwa.mjs`) that stores all the page's files in the browser's cache on the first visit. The page itself (`index.html`) comes from the network when it can, so a new version shows at the next load; the other files have a fingerprint of their content in their names and can therefore come from the cache. A manifest and icons make the site an installable app (PWA).

A.7 Development and tests

The program is developed in Node.js 24 with Vite:

`npm run dev`	the development server at `http://localhost:5173/`
`npm test`	unit tests: chemistry against RDKit, reading and writing files, complete translations
`npm run check`	the browser check (Chrome through Playwright): drawing, arrows, files, keys; in topics (`scripts/check/`), `--only drawing` runs one, `--jobs 3` three at a time
`npm run build`	builds the static site into `dist/`

`node scripts/manual-shots.mjs`	the pictures of this manual from the running program (`--en`: in English); typeset with Typst

The examples in the manual are real drawings of the program, not redrawn pictures. The script builds them from SMILES and checks every molecule through RDKit before saving, stereochemistry included.

A.8 Licence and credits

olomol is free software under the MIT License: it may be used, shared and changed, also in other programs, as long as the copyright and licence notice stays with it. The program uses **RDKit** (BSD-3-Clause, including the ring system templates © Schrödinger and its universal force field, UFF, ported to JavaScript), **Indigo** by EPAM Systems (Apache 2.0), **megane-rdkit** (BSD-3-Clause; RDKit's 3D structures as WebAssembly), **OpenChemLib** (BSD-3-Clause) and **React** (MIT). KET is the format of **Ketcher** (EPAM Systems, Apache 2.0); no Ketcher code is in the program. Compound data on request come from **PubChem** (National Library of Medicine, USA). The licence texts are in the About, credits and licences dialog. The code was written with much help from Claude, a model by Anthropic.