

MolDraw course and spectroscopy guides

The step-by-step course and the guides to reading IR, NMR and mass spectra.

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MolDraw Documentation | 2D Editor Guide

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MolDraw documentation for the current 2D editor: drawing, library, reactions, SMILES, 3D, and export.

Guide to the current MolDraw 2D editor — structures, reactions, library, SMILES, and 3D

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MolDraw is a free browser editor for 2D chemical structures, reaction schemes, and 3D viewing. This documentation matches the current editor (Home / Draw / Style ribbons, Library, and local My designs).

About This Documentation

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Documentation Structure

The [Interactive Course](#) includes:

- Getting started and Home / Draw / Style ribbons
- Drawing atoms, bonds, rings, text, and images
- Library templates, reactions, and stereochemistry
- SMILES copy/paste, download formats, and My designs
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Spectroscopy Guides: How to Read Mass, IR and NMR Spectra

<https://www.moldraw.com/guides/>

Free illustrated guides to reading mass spectra, IR spectra and $^1\text{H}/^{13}\text{C}$ NMR spectra, with annotated example spectra, worked problems and practice quizzes.

By the MolDraw chemistry team · Updated 11 Oct 2026 · Reviewed against the references listed at the end

Three step-by-step guides to the spectra you meet in organic chemistry. Each one has annotated spectra redrawn from reference data, worked examples and a practice quiz.

Quick answer: Use MS for the molecular formula, IR for functional groups, and NMR for the carbon-hydrogen framework. Combine all three to solve a structure.

On this page

1. Guides

Guides

How to read a mass spectrum Molecular ion, base peak, isotopes, fragments
How to read an IR spectrum Functional group bands, step-by-step method
How to read an NMR spectrum ^1H and ^{13}C : shift, integration, splitting, DEPT

Solve a structure: the workflow

1. MS: find M^+ and the molecular formula ([formula finder](#)).
2. Calculate the [degree of unsaturation](#).
3. IR: identify functional groups ([IR chart](#)).
4. ^{13}C and ^1H NMR: count environments, read shifts, integrals and splitting; check with [structure to NMR](#).

Practice quiz

Tap an answer to check it.

1. Which technique gives the molecular mass?

The molecular ion in a [mass spectrum](#) gives the molecular mass.

Frequently asked questions

Which spectroscopy should I learn first?

Start with IR (functional groups), then mass spectrometry (molecular formula), then [NMR](#), which gives the most structural detail.

References and data sources

- Pavia, Lampman, Kriz & Vyvyan, *Introduction to Spectroscopy*, 5th ed.
- Silverstein, Webster & Kiemle, *Spectrometric Identification of Organic Compounds*, 8th ed.

Spectra on this page are redrawn schematically from the reference data above (peak positions and approximate relative intensities) for teaching; check the original database entry before citing exact intensities.

How to Read an IR Spectrum: Step-by-Step Guide & Examples

<https://www.moldraw.com/guides/how-to-read-ir-spectrum/>

Learn how to read and interpret an IR spectrum: the 4 regions, a 6-step method, what peaks at 3000 and 1700 cm⁻¹ mean, annotated spectra of alcohols, aldehydes, ketones, esters, acids, ethers, alkynes and amines, plus a quiz.

By the MolDraw chemistry team · Updated 11 Oct 2026 · Reviewed against the references listed at the end

A practical, step-by-step method for analysing infrared spectra, with eight annotated spectra of common **functional groups** redrawn from SDBS/NIST reference data, a carbonyl table, a worked unknown and a practice quiz.

Quick answer: Check 1650–1820 cm⁻¹ for C=O, then 3200–3600 for O–H (broad) or N–H (sharper), then whether C–H bands sit above (sp²) or below (sp³) 3000 cm⁻¹, then 2100–2260 for C≡C/C≡N. Classify a carbonyl by its partner bands, and use the fingerprint region (below 1500) only to confirm.

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1. What an IR spectrum shows
2. The four regions
3. How to read it in 6 steps
4. Peaks at 3000, 1700, 1050
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What an IR spectrum shows

Infrared (IR) **spectroscopy** measures which frequencies of infrared light a molecule absorbs. Bonds vibrate (stretch and bend) at characteristic frequencies, so each functional group absorbs in a predictable region. The spectrum plots % **transmittance** (y) against

wavenumber in cm^{-1} (x, running from 4000 on the left to about 500 on the right). Absorptions appear as dips, conventionally called "peaks" or "bands".

Wavenumber is proportional to frequency and energy: stronger bonds and lighter atoms vibrate at higher wavenumbers ($\text{C}\equiv\text{C} > \text{C}=\text{C} > \text{C}-\text{C}$; O-H, N-H and C-H near 3000 because H is light).

Figure 1. Ethanol: a broad, strong O-H stretch centred near 3340 cm^{-1} (hydrogen bonding), sp^3 C-H stretches just below 3000, and a strong C-O stretch at 1048 cm^{-1} . Redrawn from SDBS/NIST data.

The four regions of an IR spectrum

Region (cm^{-1})	Bonds	What to look for
4000–2500	X-H single bonds	O-H (broad), N-H, C-H (sp 3300, sp^2 3000–3100, sp^3 2850–2960), aldehyde C-H 2720/2820
2500–2000	triple bonds, cumulated	$\text{C}\equiv\text{N}$ 2210–2260, $\text{C}\equiv\text{C}$ 2100–2260, CO_2 artefact 2350
2000–1500	double bonds	$\text{C}=\text{O}$ 1650–1820 (strong), $\text{C}=\text{C}$ 1620–1680, aromatic 1600 & 1500, N-H bend ~ 1600
1500–500	fingerprint region	C-O 1000–1300, C-N, C-X, bending modes; unique to each compound

The full band list with intensities and shapes is in our interactive [IR spectroscopy chart \(correlation table\)](#).

How to read an IR spectrum in 6 steps

1. **Check 1650–1820 cm^{-1} for C=O.** A strong, sharp band here is the single most informative peak. Absent $\rightarrow$ no carbonyl.
2. **Check 3200–3600 for O-H or N-H.** Broad and rounded $\rightarrow$ O-H (alcohol). Very broad 2500–3300 overlapping C-H $\rightarrow$ carboxylic acid O-H. One or two sharper bands $\rightarrow$ N-H (two for NH_2).
3. **Look at 3000 cm^{-1} .** Peaks just above 3000 $\rightarrow$ C-H on sp^2 carbon (alkene/aromatic); just below $\rightarrow$ sp^3 C-H; sharp 3300 $\rightarrow$ $\equiv\text{C}-\text{H}$.
4. **Scan 2100–2260** for $\text{C}\equiv\text{C}$ (weak) or $\text{C}\equiv\text{N}$ (medium, sharp).
5. **If C=O is present, classify it** using its exact position and partner bands (see table): 2720/2820 $\rightarrow$ aldehyde; 1000–1300 strong C-O $\rightarrow$ ester; broad O-H $\rightarrow$ acid; N-H $\rightarrow$ amide.
6. **Use the fingerprint region** to confirm (C-O 1000–1300; aromatic substitution 690–900) and compare with a reference spectrum.

Do not try to assign every peak. Identify the functional groups from the diagnostic regions, then use MS for the formula and NMR for the framework.

Key IR peaks: what does a peak at 3000, 1700 or 1050 cm^{-1} mean?

- **Peak at $\sim 3000 \text{ cm}^{-1}$:** C-H stretching. Below 3000 = sp^3 (alkanes, alkyl groups); above 3000 = sp^2 (alkenes, aromatics).
- **Peak at $\sim 1700 \text{ cm}^{-1}$:** a carbonyl C=O stretch, very strong. Ketones ~ 1715 , aldehydes $\sim 1725\text{--}1730$, esters $\sim 1735\text{--}1750$, carboxylic acids ~ 1710 , amides $\sim 1650\text{--}1690$, acid chlorides ~ 1800 . Conjugation lowers it by about $20\text{--}30 \text{ cm}^{-1}$.
- **Broad peak at $3200\text{--}3550 \text{ cm}^{-1}$:** hydrogen-bonded O-H of an alcohol or phenol.
- **Strong peak at $1000\text{--}1300 \text{ cm}^{-1}$:** C-O stretch (alcohols, ethers, esters).
- **Sharp peak at $\sim 2250 \text{ cm}^{-1}$:** nitrile $\text{C}\equiv\text{N}$.

IR spectra of common functional groups

Alcohol IR spectrum

Broad, strong O-H at $3200\text{--}3550 \text{ cm}^{-1}$ and a strong C-O at $1050\text{--}1150$ (primary ~ 1050 , secondary ~ 1100 , tertiary ~ 1150). See Figure 1 (ethanol).

Ketone IR spectrum

Figure 2. 2-Butanone: very strong C=O at 1717 cm^{-1} , no O-H (the weak band near 3415 is the C=O overtone), no aldehyde C-H. Redrawn from SDBS data.

Aldehyde IR spectrum (aldehyde vs ketone)

Figure 3. Butanal: C=O at $\sim 1730 \text{ cm}^{-1}$ plus the two weak aldehyde C-H bands near 2720 and 2820 cm^{-1} (Fermi resonance), which distinguish an aldehyde from a ketone.

Aldehyde vs ketone: both show a strong C=O near $1715\text{--}1730$. Only aldehydes show the C-H doublet at ~ 2720 and $\sim 2820 \text{ cm}^{-1}$; the 2720 band is the easiest to spot because nothing else absorbs there.

Ester IR spectrum

Figure 4. Ethyl acetate: C=O at 1742 cm^{-1} (higher than a ketone) and two strong C-O stretches at 1240 and 1047 cm^{-1} , the "rule of three" for esters.

Carboxylic acid IR spectrum

Figure 5. Benzoic acid: very broad O-H from 2500 to 3300 cm^{-1} (hydrogen-bonded dimer) that swallows the C-H bands, conjugated C=O at 1688 , aromatic C=C at $1603/1584$, C-O at 1292 and the broad O-H out-of-plane bend near 935 cm^{-1} .

Ether IR spectrum

Figure 6. Diethyl ether: strong C-O-C stretch near 1125 cm^{-1} and sp^3 C-H, with no O-H and no C=O. Absence of peaks is evidence too.

Alkyne IR spectrum

Figure 7. 1-Hexyne: sharp, strong $\equiv\text{C-H}$ stretch at $\sim 3310 \text{ cm}^{-1}$, weak C $\equiv$ C at ~ 2120 and $\equiv\text{C-H}$ bend near 630 cm^{-1} . Internal alkynes have no 3300 band and a very weak or absent C $\equiv$ C.

Amine IR spectrum

Figure 8. Butylamine: two medium N-H stretches (asymmetric ~ 3370 , symmetric ~ 3290 cm^{-1}) typical of NH_2 , N-H bend near 1610 and a broad N-H wag around 800 cm^{-1} . Secondary amines show one N-H band; tertiary amines none.

Aromatic compounds

C-H just above 3000 (3030 – 3100), ring C=C at ~ 1600 and ~ 1500 cm^{-1} , weak overtones 1660 – 2000 , and strong C-H out-of-plane bends at 690 – 900 cm^{-1} whose pattern indicates the substitution (monosubstituted: ~ 750 and ~ 690).

Carbonyl (C=O) positions at a glance

Compound class	C=O (cm^{-1})	Partner bands
Acid chloride	1785–1815	C-Cl ~ 730 – 550
Anhydride	1820 and 1760 (two)	C-O 1000 – 1300
Ester	1735–1750	two C-O 1000 – 1300
Aldehyde	1720–1740	C-H 2720 , 2820
Ketone	1705–1720	none
Carboxylic acid	1700–1725	O-H 2500 – 3300 very broad
Amide	1630–1690	N-H 3100 – 3500 , N-H bend 1550 – 1640
α,β -Unsaturated / aryl	subtract ~ 20 – 30	C=C 1600 – 1650

Values from Pavia *et al.* and Silverstein *et al.*; ring strain raises C=O (cyclopentanone ~ 1745 , cyclobutanone ~ 1780).

Worked example: identify the unknown

Data: formula $\text{C}_4\text{H}_8\text{O}_2$ (MS $\text{M}^{+\bullet} = 88$). IR: 2985 , 1742 (very strong), 1240 (very strong), 1047 (strong) cm^{-1} ; nothing at 3200 – 3600 .

1. Degree of unsaturation = $(2 \times 4 + 2 - 8)/2 = 1$: one ring or π bond.
2. 1742 cm^{-1} strong $\rightarrow$ C=O; no O-H $\rightarrow$ not an acid; no 2720 $\rightarrow$ not an aldehyde.
3. 1742 + two strong C-O bands $\rightarrow$ ester.
4. Candidates: ethyl acetate, methyl propanoate, propyl formate. ^1H NMR (singlet at 2.05 for $\text{CH}_3\text{C}=\text{O}$, quartet at 4.12 for OCH_2) identifies **ethyl acetate**, see the [NMR guide](#).

How to tell purity from an IR spectrum

Compare against a reference: extra bands indicate impurities. Common ones are a broad 3400 band (water or leftover alcohol), 1715 (residual acetone), 2350 (atmospheric CO_2 , an artefact) and, after a reduction, a remaining C=O band showing incomplete [reaction](#).

Next steps

Look up any band in the [IR spectroscopy chart](#). Get the molecular formula from MS ([mass spectrum guide](#), [formula finder](#)) and confirm the skeleton with [NMR](#) and the [structure-to-NMR predictor](#).

Practice quiz

Tap an answer to check it.

1. A spectrum has a strong, sharp band at 1715 cm^{-1} and nothing at 2500–3600 except C-H below 3000. The compound is most likely...

Strong C=O near 1715 with no O-H, no N-H and no aldehyde C-H → ketone.

2. A very broad band from 2500 to 3300 cm^{-1} plus a strong band at 1710 cm^{-1} indicates...

The very broad hydrogen-bonded O-H overlapping C-H, together with C=O, is the signature of a carboxylic acid.

3. Which band distinguishes an aldehyde from a ketone?

The aldehyde C-H (Fermi doublet 2720/2820) is absent in ketones.

4. A sharp, strong band at 3300 cm^{-1} and a weak band at 2120 cm^{-1} suggest...

$\equiv\text{C-H}$ at 3300 plus $\text{C}\equiv\text{C}$ at ~ 2120 → terminal alkyne.

5. Two medium bands at ~ 3370 and $\sim 3290\text{ cm}^{-1}$ indicate...

NH_2 has asymmetric and symmetric N-H stretches, giving two bands.

6. C-H peaks appear at 3030 and 2950 cm^{-1} . What does this tell you?

Above 3000 = sp^2 C-H (alkene/aromatic); below 3000 = sp^3 C-H.

Frequently asked questions

How do I read an IR spectrum?

Work left to right through the diagnostic regions: first check 1650–1820 cm^{-1} for a C=O, then 3200–3600 for O-H/N-H, then whether C-H peaks lie above or below 3000, then 2100–2260 for triple bonds. Use the fingerprint region (below 1500) only to confirm.

What does a peak at 3000 mean in IR?

C-H stretching. Peaks just below 3000 cm^{-1} come from sp^3 C-H (alkyl groups); peaks just above 3000 come from sp^2 C-H on alkenes or aromatic rings.

What IR peak is at 1700?

A carbonyl (C=O) stretch. Ketones absorb near 1715, aldehydes 1725–1730, carboxylic acids ~ 1710 , esters 1735–1750 and amides 1650–1690 cm^{-1} .

How do I interpret FTIR results?

An FTIR spectrum is read the same way as any IR spectrum: identify functional groups from characteristic bands (C=O, O-H, N-H, C-H, C≡N), then compare the whole spectrum, including the fingerprint region, with a reference library.

What does IR spectroscopy tell you?

Which functional groups a molecule contains (and which it lacks). It does not give the molecular formula or full connectivity; combine it with MS and NMR.

Can you explain IR spectroscopy in a simple way?

Chemical bonds behave like springs. Each kind of bond vibrates at its own frequency and absorbs infrared light of exactly that frequency, so the pattern of absorbed frequencies tells you which bonds are present.

What is the fingerprint region in IR?

The region below about 1500 cm⁻¹, full of complex bending and C-C/C-O stretching bands that are unique to each molecule. It is used to match an unknown to a reference spectrum.

How do you tell an aldehyde from a ketone by IR?

Both have a strong C=O near 1715–1730 cm⁻¹, but only an aldehyde shows the two weak C-H stretches near 2720 and 2820 cm⁻¹.

References and data sources

- Pavia, Lampman, Kriz & Vyvyan, *Introduction to Spectroscopy*, 5th ed., Cengage, ch. 2 (IR correlation tables).
- Silverstein, Webster & Kiemle, *Spectrometric Identification of Organic Compounds*, 8th ed., Wiley, ch. 2.
- SDBS Spectral Database for Organic Compounds (AIST, Japan): IR spectra of ethanol, 2-butanone, butanal, ethyl acetate, benzoic acid, diethyl ether, 1-hexyne, butylamine.
- NIST Chemistry WebBook, SRD 69, IR spectra (webbook.nist.gov).
- Socrates, G. *Infrared and Raman Characteristic Group Frequencies*, 3rd ed., Wiley, 2001.

Spectra on this page are redrawn schematically from the reference data above (peak positions and approximate relative intensities) for teaching; check the original database entry before citing exact intensities.

How to Read a Mass Spectrum: Step-by-Step Guide & Examples

<https://www.moldraw.com/guides/how-to-read-mass-spectrum/>

Learn how to read and interpret a mass spectrum: molecular ion, base peak, M+1/M+2 isotope patterns (Cl, Br, S), nitrogen rule, fragmentation (α -cleavage, McLafferty), losses table, worked examples and a quiz.

By the MolDraw chemistry team · Updated 11 Oct 2026 · Reviewed against the references listed at the end

This guide shows you how to interpret an electron-ionisation (EI) mass spectrum step by step: find the molecular ion, use isotope patterns and the nitrogen rule, identify the base peak and decode fragmentation. Every spectrum is annotated and redrawn from NIST reference data.

Quick answer: Find the molecular ion (highest m/z , gives the molecular mass), check isotope peaks ($M+2 = \frac{1}{3} M \rightarrow \text{Cl}$; $M+2 \approx M \rightarrow \text{Br}$), note the base peak (tallest, 100%), then subtract fragment masses from M ($15 = \text{CH}_3$, $18 = \text{H}_2\text{O}$, $29 = \text{C}_2\text{H}_5$, $43 = \text{C}_3\text{H}_7/\text{CH}_3\text{CO}$) to rebuild the structure.

On this page

1. What a mass spectrum shows
2. How to read it in 7 steps
3. Molecular ion & nitrogen rule
4. Base peak
5. Isotope patterns (Cl, Br, S)
6. Fragmentation: α -cleavage, McLafferty
7. Fragment losses table
8. Worked examples
9. Practice quiz
10. FAQ

What a mass spectrum shows

In electron-ionisation (EI) mass spectrometry, a molecule is hit by 70 eV electrons, loses one electron and becomes a radical cation, the **molecular ion, $M^{+\bullet}$** . Many molecular ions break apart; the mass spectrometer sorts the positive ions by **mass-to-charge ratio (m/z)**. Because almost all ions carry a +1 charge, m/z is simply the ion's mass.

The spectrum is a bar chart: **x-axis = m/z** , **y-axis = relative abundance**, scaled so the tallest peak is 100%. Neutral fragments (radicals and small molecules) are not detected, so you work them out from the *gaps* between peaks.

Figure 1. 2-Butanone. Molecular ion at m/z 72; base peak at m/z 43 (acylium ion $\text{CH}_3\text{C}\equiv\text{O}^+$) from α -cleavage, which loses an ethyl radical ($72 - 29 = 43$). Redrawn from NIST EI data.

How to read a mass spectrum in 7 steps

1. **Find the molecular ion ($M^{+\bullet}$).** It is usually the highest- m/z peak that is not an isotope peak. It may be small (alcohols, branched alkanes) or absent; aromatic compounds give strong $M^{+\bullet}$.

2. **Apply the nitrogen rule.** An odd M means an odd number of nitrogen atoms; an even M means zero or an even number of N.
3. **Read the isotope peaks.** M+2 about $\frac{1}{3}$ of M means one Cl; M and M+2 almost equal means one Br; M+2 about 4.4% means S. The M+1 height $\div$ 1.1% estimates the number of carbons.
4. **Identify the base peak.** The tallest peak (100%) is the most stable ion, often a clue to the main functional group.
5. **Calculate the losses from M.** M–15 (CH₃), M–18 (H₂O), M–29 (C₂H₅ or CHO), M–43 (C₃H₇ or CH₃CO)... see the table below.
6. **Look for characteristic ions:** 43 (CH₃CO⁺ or C₃H₇⁺), 77 (C₆H₅⁺), 91 (tropylium C₇H₇⁺), 105 (C₆H₅CO⁺), 31 (CH₂=OH⁺), 30 (CH₂=NH₂⁺).
7. **Propose a structure and check it** with the molecular formula, [degree of unsaturation](#), IR and NMR data.

Molecular ion peak and the nitrogen rule

The molecular ion gives the **nominal molecular mass** (using ¹²C = 12, ¹H = 1, ¹⁶O = 16, ¹⁴N = 14). With a high-resolution instrument you get the exact mass (e.g. 72.0575 for C₄H₈O) and can fix the formula with the [molecular formula finder](#) or the [exact mass calculator](#).

Nitrogen rule: nitrogen has an even mass (14) but an odd valence, so a molecule with an odd number of N atoms has an odd nominal mass. Pyridine C₅H₅N = 79; aniline C₆H₇N = 93; ethanol C₂H₆O = 46 (even, no N).

If the "highest peak" gives losses that make no sense (M–3 to M–14, or M–21 to M–25), it is probably not the molecular ion. Look for a softer ionisation method (CI, ESI) to confirm M.

What is the base peak in a mass spectrum?

The **base peak** is the tallest peak in the spectrum; all other intensities are expressed as a percentage of it. It is the most abundant ion, not necessarily the molecular ion. In 2-butanone the base peak is m/z 43 (CH₃CO⁺); in ethanol it is m/z 31 (CH₂=OH⁺); in chlorobenzene the molecular ion (m/z 112) is also the base peak, because the aromatic ring stabilises it.

Isotope patterns: M+1 and M+2 peaks (Cl, Br, S)

Element	Isotopes (natural abundance)	Pattern you see
C	¹² C 98.9%, ¹³ C 1.1%	M+1 $\approx$ 1.1% $\times$ number of C
Cl	³⁵ Cl 75.8%, ³⁷ Cl 24.2%	M : M+2 $\approx$ 3 : 1 (one Cl); 9 : 6 : 1 (two Cl)
Br	⁷⁹ Br 50.7%, ⁸¹ Br 49.3%	M : M+2 $\approx$ 1 : 1 (one Br); 1 : 2 : 1 (two Br)
S	³² S 95.0%, ³⁴ S 4.2%	M+2 $\approx$ 4.4% of M per S
N, O, F, I, P	essentially one isotope (¹⁹ F, ¹²⁷ I, ³¹ P) or small minor isotopes	no strong M+2; iodine gives a large mass gap (M–127)

Figure 2. Chlorobenzene. $M^+ \bullet$ 112 with $M+2$ at 114 one-third as tall (^{37}Cl). Loss of $\text{Cl} \bullet$ (35) gives the phenyl cation, m/z 77. Redrawn from NIST data.

Figure 3. Bromoethane. Twin molecular-ion peaks at 108 and 110 of almost equal height ($^{79}\text{Br}/^{81}\text{Br}$). Losing $\text{Br} \bullet$ gives C_2H_5^+ at m/z 29. Intensities approximate, after NIST.

Use the $M+1$ peak to estimate carbon count: $n(\text{C}) \approx (\text{height of } M+1 \div \text{height of } M) \times 100 \div 1.1$. For chlorobenzene, $6.6 \div 100 \times 100 \div 1.1 \approx 6$ carbons.

Mass spectrometry fragmentation: how molecules break

Fragmentation favours pathways that give the most stable cation (tertiary > secondary > primary; resonance-stabilised acylium, allyl, benzyl, oxonium and iminium ions).

Alpha-cleavage

The bond next to the carbon bearing a heteroatom (O, N) or next to a $\text{C}=\text{O}$ breaks. Ketones give acylium ions ($\text{R}-\text{C}\equiv\text{O}^+$); alcohols give oxonium ions ($\text{CH}_2=\text{OH}^+$ at m/z 31 for primary alcohols); amines give iminium ions ($\text{CH}_2=\text{NH}_2^+$ at m/z 30). The larger alkyl group is lost preferentially.

Figure 4. Ethanol. α -Cleavage loses $\text{CH}_3 \bullet$ ($46 - 15 = 31$) to give $\text{CH}_2=\text{OH}^+$, the base peak. $M-1$ (45) comes from loss of $\text{H} \bullet$. Redrawn from NIST data.

McLafferty rearrangement

A carbonyl compound with a hydrogen on the γ -carbon transfers that H to the $\text{C}=\text{O}$ oxygen through a six-membered transition state and loses an alkene. The product is an **even-mass** radical cation (for compounds without N): methyl ketones give m/z 58, aldehydes m/z 44, methyl esters m/z 74, carboxylic acids m/z 60.

Figure 5. 2-Hexanone. McLafferty rearrangement (loss of propene, 42) gives the enol radical cation at m/z 58; α -cleavage gives CH_3CO^+ at 43 (base) and $\text{C}_4\text{H}_9\text{CO}^+$ at 85. Intensities approximate, after NIST.

Other common patterns

- **Alkanes:** clusters 14 apart (29, 43, 57, 71...); branching weakens $M^+ \bullet$.
- **Alcohols:** weak $M^+ \bullet$, $M-18$ (water loss), α -cleavage ions.
- **Alkylbenzenes:** benzylic cleavage to the tropylium ion, m/z 91.
- **Halides:** loss of $\text{X} \bullet$ ($M-35/37$, $M-79/81$, $M-127$) and the isotope pattern.

Common fragment losses and ions (fragmentation table)

Loss from M	Neutral lost	Suggests
$M-1$	$\text{H} \bullet$	aldehydes, alcohols, amines
$M-15$	$\text{CH}_3 \bullet$	methyl group (branch, methyl ketone)
$M-17$	$\text{OH} \bullet$	carboxylic acids
$M-18$	H_2O	alcohols

Loss from M	Neutral lost	Suggests
M-26	C ₂ H ₂	aromatic rings
M-28	CO or C ₂ H ₄	ketones, phenols / ethyl groups, McLafferty
M-29	C ₂ H ₅ • or CHO•	ethyl group, aldehydes
M-31	CH ₃ O•	methyl esters, methyl ethers
M-35/37	Cl•	chlorides
M-43	C ₃ H ₇ • or CH ₃ CO•	propyl group, methyl ketones
M-45	C ₂ H ₅ O• or COOH•	ethyl esters, carboxylic acids
M-79/81	Br•	bromides
M-127	I•	iodides

Common ion (m/z)	Formula	Typical source
15, 29, 43, 57, 71	C _n H _{2n+1} ⁺	alkyl chains
30	CH ₂ =NH ₂ ⁺	primary amines
31	CH ₂ =OH ⁺	primary alcohols, ethers
43	CH ₃ CO ⁺	methyl ketones, acetates
44 / 58 / 60 / 74	McLafferty ions	aldehydes / methyl ketones / acids / methyl esters
77	C ₆ H ₅ ⁺	monosubstituted benzenes
91	C ₇ H ₇ ⁺ (tropylium)	benzyl compounds, alkylbenzenes
105	C ₆ H ₅ CO ⁺	benzoyl compounds

Worked examples

Example 1: 2-butanone (Figure 1)

M⁺• = 72 (even → 0 N). M+1 ≈ 1.1 of 25 → ≈ 4 C. Formula C₄H₈O fits 72 with one degree of unsaturation (C=O, confirmed by IR at 1715 cm⁻¹). Base peak 43 = 72 - 29: α-cleavage losing C₂H₅•. Small 57 = 72 - 15: loss of CH₃•. Both acylium ions point to CH₃-CO-CH₂CH₃.

Example 2: bromoethane (Figure 3)

Two peaks of equal height at 108 and 110 → one Br. 108 - 79 = 29 → C₂H₅. Strong m/z 29 confirms loss of Br•.

Example 3: chlorobenzene (Figure 2)

112 : 114 = 3 : 1 → one Cl. 112 - 35 = 77 → C₆H₅. A large M⁺• and m/z 77, 51 (C₄H₃⁺, loss of C₂H₂ from 77) are typical of a benzene ring.

Example 4: ethanol (Figure 4)

Even M = 46; base peak 31 = 46 - 15 shows CH₃ next to a CH₂-OH carbon (α-cleavage). Compare dimethyl ether (also 46), which gives a base peak at m/z 45 and only a weak 31, a

reminder to confirm with IR (O-H) and [NMR](#).

Check your answer with MolDraw tools

Draw a candidate in the [mass spectrum predictor](#) to see its fragments, find formulas from an [exact mass](#) with the [molecular formula finder](#), and confirm functional groups with the [IR guide](#) and the [IR chart](#). For the C-H framework, continue with [how to read an NMR spectrum](#).

Practice quiz

Tap an answer to check it.

1. A spectrum shows peaks at m/z 156 and 158 of nearly equal height. Which element is present?

^{79}Br and ^{81}Br are almost 1:1, giving M and $M+2$ of equal height (bromobenzene, $\text{C}_6\text{H}_5\text{Br}$, $M = 156$).

2. The molecular ion is at m/z 73. What can you conclude?

Nitrogen rule: odd nominal mass $\rightarrow$ odd number of N atoms (e.g. $\text{C}_4\text{H}_{11}\text{N}$, butylamine).

3. A methyl ketone gives a strong even-mass peak at m/z 58. Which process forms it?

McLafferty rearrangement of a methyl ketone with a γ -hydrogen gives the enol radical cation $\text{CH}_2=\text{C}(\text{OH})\text{CH}_3^+\bullet$, m/z 58.

4. A peak at $M-18$ most likely indicates...

Loss of 18 mass units = H_2O , typical of alcohols.

5. An alkylbenzene shows a base peak at m/z 91. This ion is...

Benzylic cleavage gives C_7H_7^+ , which rearranges to the aromatic tropylium ion, m/z 91.

6. $M = 100$ and $M+1 = 6.6$ (relative). Roughly how many carbons?

$6.6 \div 100 \times 100 \div 1.1 \approx 6$ carbons.

Frequently asked questions

How do I interpret a mass spectrum?

Find the molecular ion (highest m/z , not an isotope peak), apply the nitrogen rule, read $M+1/M+2$ isotope peaks for C, Cl, Br and S, identify the base peak, then work out neutral losses from M (e.g. $M-15 = \text{CH}_3$, $M-18 = \text{H}_2\text{O}$) and match characteristic ions such as 43, 77 and 91.

What is the base peak in a mass spectrum?

The tallest peak, set to 100% relative abundance. It is the most abundant (usually most stable) ion and is often a fragment rather than the molecular ion.

What is the difference between the molecular ion and the base peak?

The molecular ion $M^{+\bullet}$ is the intact molecule minus one electron and gives the molecular mass. The base peak is simply the most intense peak; sometimes they are the same peak (e.g. chlorobenzene, m/z 112).

How do you read a mass spectrometry chart?

The x-axis is the mass-to-charge ratio (m/z) and the y-axis is the relative abundance (%) compared with the base peak. Each bar is an ion; differences between bars correspond to neutral fragments that were lost.

What does an M+2 peak mean?

A peak two units above M from a heavier isotope. M+2 about one-third of M indicates chlorine; M and M+2 nearly equal indicates bromine; about 4% suggests sulfur.

Can you explain mass spectrometry to a beginner?

A mass spectrometer turns molecules into charged ions, breaks some of them into pieces and weighs each piece. The resulting bar chart tells you the mass of the whole molecule and of its fragments, which you piece together like a puzzle to deduce the structure.

What is the nitrogen rule?

A compound with an odd nominal molecular mass contains an odd number of nitrogen atoms; an even mass means zero or an even number of nitrogens.

References and data sources

- NIST Chemistry WebBook, SRD 69: EI mass spectra of 2-butanone, bromoethane, chlorobenzene, ethanol and 2-hexanone (webbook.nist.gov).
- SDBS Spectral Database for Organic Compounds, AIST Japan.
- McLafferty, F. W.; Tureček, F. *Interpretation of Mass Spectra*, 4th ed., University Science Books, 1993.
- Pavia, Lampman, Kriz & Vyvyan, *Introduction to Spectroscopy*, 5th ed., Cengage, ch. 8.
- Silverstein, Webster & Kiemle, *Spectrometric Identification of Organic Compounds*, 8th ed., Wiley, ch. 1.
- Isotope abundances: IUPAC CIAAW, isotopic compositions of the elements.

Spectra on this page are redrawn schematically from the reference data above (peak positions and approximate relative intensities) for teaching; check the original database entry before citing exact intensities.

How to Read NMR Spectra (^1H & ^{13}C): Shifts, Splitting, DEPT

<https://www.moldraw.com/guides/how-to-read-nmr-spectrum/>

Learn how to read and interpret ^1H and ^{13}C NMR spectra: chemical shift tables, integration, $n+1$ splitting, coupling constants, equivalence, DEPT-90/135, annotated spectra, worked

examples and a practice quiz.

By the MolDraw chemistry team · Updated 11 Oct 2026 · Reviewed against the references listed at the end

A complete, illustrated guide to interpreting proton and carbon-13 NMR: what each feature means, reference tables, annotated spectra with expanded multiplets and integrals, DEPT, three worked unknowns and a quiz.

Quick answer: Count the signals (proton environments), read each chemical shift (e.g. 0.9–1.8 alkyl, 3.3–4.5 next to O, 6.5–8.5 aromatic, 9–10 aldehyde), use the integrals for the number of H, and apply the $n+1$ rule to the splitting to find neighbouring H. In ^{13}C NMR each line is one carbon environment; DEPT tells you CH, CH_2 or CH_3 .

On this page

1. What an NMR spectrum shows
2. How to read ^1H NMR in 6 steps
3. Chemical shift table
4. Integration
5. Splitting & the $n+1$ rule
6. Coupling constants
7. Equivalence: how many signals?
8. Reading ^{13}C NMR
9. DEPT-90 / DEPT-135
10. Worked examples
11. Solvent, water & D_2O
12. Practice quiz

What an NMR spectrum shows

Nuclear magnetic resonance (NMR) [spectroscopy](#) detects nuclei such as ^1H and ^{13}C in a strong magnetic field. Each chemically different nucleus resonates at a slightly different frequency, reported as the **chemical shift δ in ppm** relative to tetramethylsilane (TMS, $\delta = 0$). The x-axis runs from high δ on the left (*downfield*, deshielded) to low δ on the right (*upfield*, shielded).

A ^1H NMR spectrum gives four pieces of information: **(1) number of signals** = number of proton environments, **(2) chemical shift** = type of environment, **(3) integration** = relative number of H, **(4) splitting** = number of neighbouring H.

Figure 1. Ethyl acetate: three signals. a: OCH_2 quartet at 4.12 (2H, $J = 7.1$ Hz); b: $\text{CH}_3\text{C}=\text{O}$ singlet at 2.05 (3H); c: CH_3 triplet at 1.26 (3H). Insets show each multiplet expanded; the stepped line is the integral (2 : 3 : 3). Data consistent with SDBS.

How to read a ^1H NMR spectrum in 6 steps

1. **Get the formula and degree of unsaturation** from MS ([formula finder](#)) and the [degree of unsaturation calculator](#).

2. **Count the signals** → number of different H environments (equivalent protons give one signal).
3. **Read each chemical shift** with the table below (e.g. 0.9–1.8 alkyl, 2.0–2.7 next to C=O or aromatic ring, 3.3–4.5 next to O or halogen, 6.5–8.5 aromatic, 9–10 aldehyde).
4. **Use the integrals** to find the ratio of H, then scale to the formula's total H.
5. **Read the splitting (n+1 rule)**: a signal split into n+1 lines has n equivalent neighbouring H on adjacent carbons.
6. **Assemble fragments** (e.g. a 2H quartet + 3H triplet = ethyl group CH₂CH₃), then check the full structure with the [structure-to-NMR predictor](#).

Chemical shift: ¹H NMR chemical shift table

Electronegative atoms and π systems pull electron density away from a proton (deshielding), moving it downfield (higher δ). Aromatic and aldehyde protons are further deshielded by ring currents and C=O anisotropy.

Proton type	δ (ppm)	Example
TMS reference	0.0	Si(CH ₃) ₄
Alkyl C-H (CH ₃ , CH ₂ , CH)	0.9–1.8	CH ₃ of ethyl, 0.9–1.3
Allylic, benzylic, α to C=O	1.7–2.7	CH ₃ C=O 2.0–2.2; ArCH ₃ 2.3
Alkyne ≡C-H	2.0–3.0	terminal alkyne ~2.5
C-H next to N	2.2–2.9	CH ₂ NH ₂ ~2.7
C-H next to halogen	2.5–4.5	CH ₃ Cl 3.05; (CH ₃) ₂ CHCl 4.17
C-H next to O (alcohol, ether, ester)	3.3–4.5	OCH ₃ 3.3–3.9; OCH ₂ of ester ~4.1
Vinyllic =C-H	4.5–6.5	alkenes
Aromatic Ar-H	6.5–8.5	benzene 7.36
Aldehyde CHO	9–10	~9.7
Carboxylic acid COOH	10–13 (broad)	~11–12
Alcohol O-H / amine N-H	0.5–5 (variable, broad)	depends on solvent and concentration
Phenol O-H	4–8	variable

Integration: how many protons?

The area under each signal is proportional to the number of protons producing it. Spectrometers display an integral curve (the stepped line in the figures) or a number under each peak. Integrals give *ratios*: for ethyl acetate the steps are 2 : 3 : 3, which already adds up to the 8 H of C₄H₈O₂. If the ratio adds up to fewer H than the formula, multiply (e.g. 1 : 1.5 → 2 : 3).

Splitting and the n+1 rule

Protons on adjacent carbons (three bonds apart, H-C-C-H) couple through the bonding electrons. A proton with **n equivalent neighbouring protons** is split into **n + 1 lines** with intensities from Pascal's triangle. Equivalent protons do not split each other, and O-H/N-H protons usually do not couple because they exchange rapidly.

Neighbours (n)	Lines	Name	Intensities
0	1	singlet (s)	1
1	2	doublet (d)	1:1
2	3	triplet (t)	1:2:1
3	4	quartet (q)	1:3:3:1
4	5	quintet (pentet)	1:4:6:4:1
5	6	sextet	1:5:10:10:5:1
6	7	septet	1:6:15:20:15:6:1

Figure 2. 2-Chloropropane: the CH next to Cl has six equivalent neighbours → septet at 4.17 ppm (1H); the two equivalent CH₃ groups have one neighbour → doublet at 1.52 ppm (6H). Both share J = 6.5 Hz.

Partner check: coupled signals share the same J value. A quartet and a triplet with the same J = an ethyl group; a septet and a 6H doublet = an isopropyl group.

Coupling constants (J values)

The spacing between lines of a multiplet, in hertz, is the coupling constant J. It does not change with magnet strength, so it tells you about geometry.

Relationship	Typical J (Hz)
Vicinal H-C-C-H, free rotation (sp ³)	6-8
Alkene, trans	11-18
Alkene, cis	6-14
Alkene, geminal (=CH ₂)	0-3
Aromatic ortho	6-10 (≈ 8)
Aromatic meta	1-3
Aromatic para	0-1
Aldehyde CHO-CH	1-3

When a proton has two different sets of neighbours with different J values the n+1 rule is applied twice, giving a doublet of doublets (dd), doublet of triplets (dt), and so on. Overlapping, complex patterns are reported as multiplets (m).

Chemical equivalence: how many signals?

Protons are equivalent if they are interchanged by symmetry (a mirror plane, a rotation axis) or by fast rotation. Replace each H in turn with a test group "X": if you get the same compound, those H are equivalent. Examples: ethane (1 signal), propane (2), 2-chloropropane (2), ethyl acetate (3), toluene (4: CH₃ plus ortho, meta and para ring H, although the ring H often overlap). Diastereotopic CH₂ protons next to a stereocentre are not equivalent and can give separate signals.

How to read a ¹³C NMR spectrum

Routine ¹³C spectra are **proton-decoupled**, so every unique carbon gives a single line; there is no splitting, and peak heights are *not* reliable for counting (quaternary carbons are weak). Count the lines to get the number of carbon environments and use the shift ranges:

Carbon type	δ (ppm)
sp ³ alkyl (CH ₃ , CH ₂ , CH)	0-50
C-N	30-65
C-O (alcohols, ethers, esters)	50-90
Alkyne C≡C	65-90
Alkene C=C	100-150
Aromatic C	110-160
Nitrile C≡N	115-125
Acid, ester, amide C=O	160-185
Aldehyde, ketone C=O	190-220

Figure 3. Ethyl acetate: four carbons, four lines. Ester C=O 171.1, OCH₂ 60.5, CH₃C=O 21.0, CH₃ 14.2 ppm. The quaternary C=O is weaker.

Figure 4. 2-Butanone: ketone C=O at 209.3 ppm (above 200 → ketone or aldehyde), CH₂ 36.9, CH₃CO 29.4, CH₃ 7.9 ppm.

DEPT basics: CH, CH₂ or CH₃?

DEPT (Distortionless Enhancement by Polarization Transfer) experiments edit a ¹³C spectrum by the number of attached H. **DEPT-90** shows only CH carbons. **DEPT-135** shows CH and CH₃ pointing up and CH₂ pointing down. Quaternary carbons (no H) are absent from both, so comparing with the normal ¹³C spectrum identifies them.

Figure 5a. Ethylbenzene ¹³C: ipso C 144.2, three aromatic CH (128.4, 127.9, 125.7), CH₂ 28.9, CH₃ 15.6 ppm.

Figure 5b. DEPT-135: aromatic CH and CH₃ up, CH₂ (28.9) down, ipso carbon (144.2) missing because it carries no H.

Figure 5c. DEPT-90: only the three aromatic CH carbons appear.

Worked examples

Example 1: C₄H₈O, IR 1717 cm⁻¹

Figure 6. Quartet 2.44 (2H, J 7.3), singlet 2.14 (3H), triplet 1.06 (3H, J 7.3).

DoU = 1 and IR shows a ketone C=O. The 2H quartet and 3H triplet share J = 7.3 Hz → an ethyl group; the CH₂ at 2.44 is next to C=O. The 3H singlet at 2.14 is a methyl on C=O with no neighbours. Answer: **2-butanone**, CH₃COCH₂CH₃, confirmed by four ¹³C lines including 209 ppm (Figure 4).

Example 2: C₈H₁₀

Figure 7. Multiplet 7.15–7.31 (5H), quartet 2.65 (2H, J 7.6), triplet 1.24 (3H, J 7.6).

DoU = 4 → a benzene ring is likely. 5 aromatic H → monosubstituted ring. Quartet + triplet = ethyl; CH₂ at 2.65 is benzylic. Answer: **ethylbenzene**. DEPT (Figure 5) shows one quaternary aromatic C, three CH, one CH₂ and one CH₃.

Example 3: C₃H₇Cl

Two signals: 1H septet at 4.17 and 6H doublet at 1.52 (Figure 2). Septet + 6H doublet = isopropyl; CH at 4.17 bears Cl. Answer: **2-chloropropane** (1-chloropropane would give three signals: t 3.5, sextet 1.8, t 1.0).

Solvent, water and D₂O

Spectra are run in deuterated solvents (CDCl₃, DMSO-d₆, D₂O) so the solvent does not swamp the sample; residual CHCl₃ appears at 7.26 ppm. Water shows up as a singlet at about 1.56 ppm in CDCl₃ (3.33 in DMSO-d₆). Shaking the sample with a drop of D₂O exchanges O–H and N–H protons for deuterium, so their signals disappear, a quick way to identify them.

Practise with MolDraw

Draw any structure and predict its spectrum with [structure to NMR](#) or [SMILES to NMR](#); in the editor the [NMR Analyser plugin](#) adds COSY, HSQC and HMBC. Combine NMR with the [IR guide](#), [IR chart](#) and the [mass spectrum guide](#) to solve full structures.

Practice quiz

Tap an answer to check it.

1. A 2H quartet and a 3H triplet with the same J value indicate...

CH₂ (3 neighbours → quartet) next to CH₃ (2 neighbours → triplet) = ethyl.

2. A proton has six equivalent neighbours. Its signal is a...

n + 1 = 7 lines = septet, as for the CH of an isopropyl group.

3. A singlet at 9.7 ppm most likely belongs to...

Aldehyde protons appear at 9–10 ppm.

4. How many ^1H NMR signals does 2-chloropropane give?

The two CH_3 groups are equivalent (one signal) plus the CH: two signals.

5. In a DEPT-135 spectrum, a negative peak is a...

DEPT-135: CH_2 down; CH and CH_3 up; quaternary absent.

6. A ^{13}C line at 208 ppm indicates...

Above ~ 190 ppm $\rightarrow$ aldehyde or ketone carbonyl.

7. Integrals of 1 : 1.5 for a compound with 10 H in two signals correspond to...

1 : 1.5 = 2 : 3; scaled to 10 H gives 4H and 6H.

Frequently asked questions

How do I interpret a ^1H NMR spectrum?

Count the signals (proton environments), read each chemical shift to identify the environment, use the integrals for the number of H, and use the splitting ($n+1$ rule) to find the number of neighbouring H. Then join the fragments into a structure consistent with the molecular formula.

How do you interpret a ^{13}C NMR spectrum?

Each line is a unique carbon environment (spectra are proton-decoupled, so there is no splitting). Use shift ranges: 0–50 sp^3 , 50–90 C–O, 100–160 alkene/aromatic, 160–185 acid/ester/amide C=O, 190–220 aldehyde/ketone C=O. DEPT tells you how many H each carbon carries.

What does an NMR peak at 0 ppm mean?

$\delta = 0$ is the reference signal of tetramethylsilane (TMS) added as an internal standard. It is not part of your compound.

What are 5 peaks on NMR called?

A quintet (or pentet), intensities 1:4:6:4:1, from a proton with four equivalent neighbouring protons.

What are 6 peaks called in NMR?

A sextet, intensities 1:5:10:10:5:1, from a proton with five equivalent neighbours (e.g. the middle CH_2 of a propyl group).

What is the $n+1$ rule?

A proton with n equivalent neighbouring protons on adjacent carbons appears as $n + 1$ lines: 0 $\rightarrow$ singlet, 1 $\rightarrow$ doublet, 2 $\rightarrow$ triplet, 3 $\rightarrow$ quartet.

Why do we use D₂O in NMR?

D₂O is a deuterated solvent with no ¹H signal, and a "D₂O shake" exchanges O-H and N-H protons for deuterium so their peaks disappear, identifying them.

Does water show up on NMR?

Yes. Traces of water give a singlet near 1.56 ppm in CDCl₃, 3.33 ppm in DMSO-d₆ and 4.79 ppm in D₂O (as HDO).

What does DEPT-135 show?

CH and CH₃ carbons as positive peaks, CH₂ carbons as negative peaks; quaternary carbons are absent.

References and data sources

- Pavia, Lampman, Kriz & Vyvyan, *Introduction to Spectroscopy*, 5th ed., Cengage, ch. 5-7.
- Silverstein, Webster & Kiemle, *Spectrometric Identification of Organic Compounds*, 8th ed., Wiley, ch. 3-4.
- SDBS Spectral Database for Organic Compounds (AIST): ¹H/¹³C NMR of ethyl acetate, 2-butanone, 2-chloropropane, ethylbenzene.
- Fulmer, G. R. *et al.* "NMR Chemical Shifts of Trace Impurities", *Organometallics* 2010, 29, 2176 (water and solvent residual peaks).
- Reich, H. J. Structure Determination Using NMR, University of Wisconsin (chemical shift and coupling constant tables).

Spectra on this page are redrawn schematically from the reference data above (peak positions and approximate relative intensities) for teaching; check the original database entry before citing exact intensities.

Learn MolDraw: free hands-on chemistry drawing lessons

<https://www.moldraw.com/learn/>

Short hands-on lessons for the MolDraw editor. Watch, then draw in the real editor with instant checks.

Short hands-on lessons. Watch a quick animation, then try it in the real editor. The page checks your drawing and gives hints.

0 of 38 chapters done

Chapters

Chapters for this level are coming soon.

1. [How to draw a benzene ring and phenol](#) Draw a benzene ring, then add an OH group to make phenol. The editor checks each step as you draw. Beginner 5 min · 2 steps

2. [How to draw double, triple and wedge bonds](#) Pick a bond type from the bond menu, then click a bond to change it. Press 1, 2 or 3 for single, double or triple bonds. Beginner 5 min · 3 steps
3. [How to add atoms, elements and formal charges](#) Pick an element in the atom palette and click an atom to change it. Use the plus and minus tools to add charges. Beginner 5 min · 3 steps
4. [How to draw lone pairs and radicals](#) Pick the lone pair tool and click an atom to add a pair of dots. Pick Free radical in the same menu to add a single dot. Beginner 4 min · 3 steps
5. [How to draw rings, chairs and fused rings](#) Pick a ring in the ring bar and click the canvas. Click a ring bond with benzene to fuse a second ring. Pick Chair to draw a cyclohexane chair. Beginner 5 min · 3 steps
6. [How to use R groups and labels like Ph and COOH](#) Pick the atom label tool, click an atom and type a label such as Ph, COOH or R1. Press Enter to finish. Beginner 4 min · 3 steps
7. [How to draw stereochemistry with wedge and hash bonds](#) Change a bond at a stereocenter to a wedge or hash bond. Turn on R and S labels in Settings to see the configuration. Beginner 5 min · 3 steps
8. [How to draw a reaction scheme with arrows](#) Draw the starting material, add a reaction arrow, draw the product, then type the reagents above the arrow. Beginner 6 min · 4 steps
9. [How to draw curved arrow mechanisms](#) Draw the species, add lone pairs, then draw a curved arrow from the electrons to the atom that receives them. Beginner 6 min · 4 steps
10. [How to turn a name or SMILES into a structure](#) Click Paste SMILES and type a SMILES string, or type a name in the PubChem search box. MolDraw draws the structure for you. Beginner 4 min · 3 steps
11. [How to find the formula, weight and IUPAC name](#) Select your molecule and click Info. The panel shows the name, formula and weight. Click Copy IUPAC to copy the name. Beginner 4 min · 3 steps
12. [How to view a molecule in 3D](#) Click Show 3D viewer at the bottom of the atom palette. Drag to rotate the model. Use 3D Clean Up to pose the 2D drawing. Beginner 4 min · 3 steps
13. [How to export a structure for a paper or slides](#) Click Download and pick SVG or PDF for papers, or PNG for slides. Beginner 4 min · 3 steps
14. [How to predict an NMR spectrum from a structure](#) Draw the molecule and copy its SMILES. Paste it into the free MolDraw NMR predictor, or use the NMR Analyser plugin with a free account. Beginner 4 min · 2 steps
15. [How to change atom colours and colour a structure](#) Turn on element colours in Settings. To colour part of a molecule, select it and pick a colour in Color and style. Beginner 4 min · 3 steps
16. [How to change font size and atom label style](#) Open Color and style, then Atoms. Pick a label font and a label size. All atom labels update at once. Beginner 4 min · 3 steps
17. [How to set bond length, line width and bond style](#) Open Color and style, then Bonds. Set Bond thickness for line width and Bond length for size. Beginner 4 min · 3 steps

18. [How to use themes and ball and stick style](#)Open Color and style and set Look to Ball and stick. Set it back to Default for the plain line style.Beginner 3 min · 3 steps
19. [How to align, arrange and space out structures](#)Select several structures. Use the align buttons above the selection to line them up, then Distribute to space them evenly.Beginner 4 min · 3 steps
20. [How to make publication quality structure figures](#)Pick the ACS Document 1996 style in Settings, Style presets. Then download a PDF or SVG for your paper.Beginner 5 min · 3 steps
21. [How to clean up a chemical structure](#)Draw toluene, then click Cleanup structure. MolDraw evens out bond lengths and angles in one click.Beginner 3 min · 2 steps
22. [How to use ring templates and the structure library](#)Place a ring from the ring bar, then add a ready-made amino acid from the Library.Beginner 4 min · 2 steps
23. [How to draw polymer repeat unit brackets](#)Draw one ethylene unit, then drag polymer brackets around it to show polyethylene.Beginner 3 min · 2 steps
24. [How to add text and shapes to a drawing](#)Add a text label, then a rectangle and a circle from the Draw tab.Beginner 4 min · 2 steps
25. [How to use keyboard shortcuts to draw faster](#)Use Ctrl+A, Delete and Ctrl+Z to select, clear and undo in seconds.Beginner 3 min · 3 steps
26. [How to draw lab apparatus and glassware](#)Open the Draw tab, pick Glassware and drag a flask onto the canvas. Then label it.Beginner 3 min · 2 steps
27. [How to add ligands and functional groups](#)Open the Library, switch to Ligands and add pyridine and triphenylphosphine.Beginner 3 min · 2 steps
28. [How to search PubChem by name or CAS number](#)Type a name or a CAS number in the PubChem box. MolDraw draws the structure for you.Beginner 3 min · 2 steps
29. [How to export MOL, SVG and other file formats](#)Draw benzene, then download it as a MOL file and as an SVG image.Beginner 3 min · 3 steps
30. [How to open the AI chemistry assistant](#)Open AI chat from the tools row. Ask it to draw a molecule from a name or a description.Beginner 2 min · 2 steps
31. [How to sketch structures with Smart Draw](#)Smart Draw turns freehand strokes into bonds, rings and labels. Draw cyclohexane here, then sketch it in the full editor.Beginner 4 min · 2 steps
32. [How to predict a mass spectrum](#)Draw ethanol here, then ask the AI Spectroscopy plugin for its mass spectrum in the full editor.Beginner 4 min · 2 steps
33. [How to show an electrostatic potential map](#)Draw phenol here, then colour its 3D surface by charge with the MEP plugin.Beginner 4 min · 2 steps
34. [How to compare two molecules for similarity](#)Draw benzene and toluene, then compare them with the Compare plugin.Beginner 4 min · 2 steps
35. [How to look up a molecule in ChEMBL](#)Load aspirin here, then find its targets and activity data with the ChEMBL plugin.Beginner 4 min · 2 steps
36. [How to view a protein structure from the PDB](#)Open the 3D viewer here, then load a protein by its PDB ID in the full editor.Beginner 4 min · 3 steps
37. [How to map atoms in a reaction](#)Draw a simple reaction here, then number matching atoms with Automap in the full editor.Beginner 4 min · 2 steps
38. [How to use Community, Dashboard and your profile](#)Sign in to save designs online, share them in Community and manage them from your Dashboard.Beginner 3 min · 2

steps

How it works

Each chapter has a short animation and an exercise. Open **1. Watch demo** first. Then open **2. Try in editor** and draw in the full MolDraw editor. Each step ticks by itself when your drawing is right. Your progress saves in this browser.

How to add atoms, elements and formal charges | Learn MolDraw

<https://www.moldraw.com/learn/how-to-add-atoms-elements-and-formal-charges/>

Pick an element in the atom palette and click an atom to change it. Use the plus and minus tools to add charges.

Beginner 5 min 3 steps

Short answer: Pick an element in the atom palette and click an atom to change it. Use the plus and minus tools to add charges.

You will learn to: Change carbon to O or N; Grow a chain from an atom; Add a positive charge.

1 Watch demo 2 Try in editor

Watch the demo

Atoms and charges in about 20 seconds.

The steps in text

Step 1: Draw ethanol

1. Pick the single bond tool. Click an empty spot to draw one bond.
2. Click **O** in the atom palette. Click the left atom.
3. Click **C** in the palette. Pick the bond tool again. Click the right atom to add one more carbon.

Step 2: Change O to N

1. Click **N** in the atom palette.
2. Click the O atom.

Step 3: Add a positive charge to N

1. Pick the **+** tool in the left rail.
2. Click the N atom.

Try it in the editor

Chapter complete

Next: How to draw lone pairs and radicals

[Next chapter](#)

The full MolDraw editor opens here. It loads when you open this tab.

Questions and answers

How do I change an atom to another element?

Pick the element in the atom palette, then click the atom.

How do I add a charge to an atom?

Pick the plus or minus tool in the left rail and click the atom.

Where is the periodic table?

Click the grid button at the bottom of the atom palette.

For more detail, read [the guide in the docs](#).

How to add ligands and functional groups | Learn MolDraw

<https://www.moldraw.com/learn/how-to-add-ligands-and-functional-groups-from-the-library/>

Open the Library, switch to Ligands and add pyridine and triphenylphosphine.

Beginner 3 min 2 steps

Short answer: Open the Library, switch to Ligands and add pyridine and triphenylphosphine.

You will learn to: Open the Ligands tab; Place two ligands.

1 Watch demo 2 Try in editor

Watch the demo

Ligands in about 15 seconds.

The steps in text

Step 1: Add pyridine

1. Click **Library** at the right end of the ring bar.
2. Click the **Ligands** tab. Click **Pyridine**.
3. Click an empty spot on the canvas.

Step 2: Add triphenylphosphine

1. Open the Library again. Pick **Ligands**.
2. Click **Triphenylphosphine**. Click an empty spot.

Try it in the editor

Chapter complete

Next: How to search PubChem by name or CAS number

[Next chapter](#)

The full MolDraw editor opens here. It loads when you open this tab.

Questions and answers

How do I attach a ligand to a metal?

Pick the ligand, then click the metal atom. MolDraw connects it.

Where are functional groups?

Use the R-groups tab, or type a label such as COOH with the atom label tool.

For more detail, read [the guide in the docs](#).

How to add text and shapes to a drawing | Learn MolDraw

<https://www.moldraw.com/learn/how-to-add-text-and-shapes-to-a-chemical-drawing/>

Add a text label, then a rectangle and a circle from the Draw tab.

Beginner 4 min 2 steps

Short answer: Add a text label, then a rectangle and a circle from the Draw tab.

You will learn to: Type a text label; Draw shapes from the Draw tab.

1 Watch demo 2 Try in editor

Watch the demo

Text and shapes in about 20 seconds.

The steps in text

Step 1: Add a label

1. Pick the **Text** tool (the T in the tools row).
2. Click an empty spot. Type **Figure 1**. Press Esc.

Step 2: Draw two shapes

1. Click the **Draw** tab at the top.
2. Pick **Rectangle**. Drag on the canvas.
3. Pick **Circle**. Drag again.

Try it in the editor

Chapter complete

Next: How to use keyboard shortcuts to draw faster

[Next chapter](#)

The full MolDraw editor opens here. It loads when you open this tab.

Questions and answers

Can I add images?

Yes. Use Image in the Draw tab. PNG, JPEG, WebP, GIF and SVG work.

How do I change text size?

Select the text and use Color and style.

For more detail, read [the guide in the docs](#).

How to align, arrange and space out structures | Learn MolDraw

<https://www.moldraw.com/learn/how-to-align-arrange-and-distribute-structures-on-the-canvas/>

Select several structures. Use the align buttons above the selection to line them up, then Distribute to space them evenly.

Beginner 4 min 3 steps

Short answer: Select several structures. Use the align buttons above the selection to line them up, then Distribute to space them evenly.

You will learn to: Draw three separate pieces; Align them on one line; Space them evenly.

1 Watch demo 2 Try in editor

Watch the demo

Align and distribute in about 15 seconds.

The steps in text

Step 1: Draw three separate bonds

1. Pick the single bond tool.
2. Click three empty spots at different heights.

Step 2: Align them on one line

1. Press Esc. Then press Ctrl+A to select all.
2. Click **Align on horizontal centres** in the bar above the selection.

Step 3: Space them evenly

1. Keep them selected.
2. Click **Distribute horizontally**.

Try it in the editor

Chapter complete

Next: How to make publication quality structure figures

[Next chapter](#)

The full MolDraw editor opens here. It loads when you open this tab.

Questions and answers

How do I line up two molecules?

Select both, then click an align button above the selection.

How do I space out a reaction scheme?

Select the items and click Distribute horizontally.

Can I align text and arrows too?

Yes. Align works on any selected objects.

For more detail, read [the guide in the docs](#).

How to change atom colours and colour a structure | Learn MolDraw

<https://www.moldraw.com/learn/how-to-change-atom-colours-and-colour-structures-in-moldraw/>

Turn on element colours in Settings. To colour part of a molecule, select it and pick a colour in Color and style.

Beginner 4 min 3 steps

Short answer: Turn on element colours in Settings. To colour part of a molecule, select it and pick a colour in Color and style.

You will learn to: Turn on element colours; Select a molecule; Colour it red.

1 Watch demo 2 Try in editor

Watch the demo

Colours in about 20 seconds.

The steps in text

Step 1: Draw ethanol

1. Draw one bond. Change the left atom to **O**.
2. Click **C** in the palette. Then click the right atom with the bond tool.

Step 2: Turn on element colours

1. Click **Settings** (the gear).
2. Turn on **Color atom labels by element**. Close Settings.

Step 3: Colour the molecule red

1. Press **Ctrl+A** to select all.
2. Click **Color and style** (the palette button).
3. Click the red swatch.

Try it in the editor

Chapter complete

Next: How to change font size and atom label style

[Next chapter](#)

The full MolDraw editor opens here. It loads when you open this tab.

Questions and answers

How do I colour one part of a molecule?

Select that part, then pick a colour in Color and style.

How do I colour atoms by element?

Open Settings and turn on Color atom labels by element.

Do colours stay in exports?

Yes. Colours stay in SVG, PDF and PNG files.

For more detail, read [the guide in the docs](#).

How to change font size and atom label style | Learn MolDraw

<https://www.moldraw.com/learn/how-to-change-font-size-and-atom-label-style-in-chemical-drawings/>

Open Color and style, then Atoms. Pick a label font and a label size. All atom labels update at once.

Beginner 4 min 3 steps

Short answer: Open Color and style, then Atoms. Pick a label font and a label size. All atom labels update at once.

You will learn to: Open the Atoms style section; Change the label font; Change the label size.

1 Watch demo2 Try in editor

Watch the demo

Fonts in about 20 seconds.

The steps in text

Step 1: Draw ethanol

1. Draw one bond. Change the left atom to **O**.
2. Click **C** in the palette. Then click the right atom with the bond tool.

Step 2: Change the label font to Arial

1. Click **Color and style**. Open **Atoms**.
2. Set **Label font** to **Arial**.

Step 3: Set the label size to 28 pt

1. In the same section, set **Label size** to **28 pt**.

Try it in the editor

Chapter complete

Next: How to set bond length, line width and bond style

[Next chapter](#)

The full MolDraw editor opens here. It loads when you open this tab.

Questions and answers

How do I make atom labels bigger?

Open Color and style, then Atoms, and raise Label size.

Which fonts can I use?

Times New Roman, Arial, Helvetica, Inter and several more.

Does the font change my exports?

Yes. SVG, PDF and PNG use the font you pick.

For more detail, read [the guide in the docs](#).

How to clean up a chemical structure | Learn MolDraw

<https://www.moldraw.com/learn/how-to-clean-up-a-chemical-structure-drawing/>

Draw toluene, then click Cleanup structure. MolDraw evens out bond lengths and angles in one click.

Beginner 3 min 2 steps

Short answer: Draw toluene, then click Cleanup structure. MolDraw evens out bond lengths and angles in one click.

You will learn to: Draw toluene from a benzene ring; Use the Cleanup structure button.

1 Watch demo 2 Try in editor

Watch the demo

Cleanup in about 15 seconds.

The steps in text

Step 1: Draw toluene

1. Click the benzene button in the ring bar. Click the canvas.
2. Pick the single bond tool. Click the top atom of the ring.

Step 2: Clean up the drawing

1. Click **Cleanup structure** in the tools row. It is the magic wand button.

Try it in the editor

Chapter complete

Next: How to use ring templates and the structure library

[Next chapter](#)

The full MolDraw editor opens here. It loads when you open this tab.

Questions and answers

What does Cleanup structure do?

It redraws your structure with even bond lengths and standard angles. Atoms and bonds stay the same.

Can I undo a cleanup?

Yes. Press Ctrl+Z.

For more detail, read [the guide in the docs](#).

How to compare two molecules for similarity | Learn MolDraw

<https://www.moldraw.com/learn/how-to-compare-two-molecules-for-similarity/>

Draw benzene and toluene, then compare them with the Compare plugin.

Beginner 4 min 2 steps

Short answer: Draw benzene and toluene, then compare them with the Compare plugin.

You will learn to: Draw two related molecules; Read a Tanimoto score.

1 Watch demo 2 Try in editor

Watch the demo

Two molecules in about 15 seconds.

The steps in text

Step 1: Draw benzene and toluene

1. Place a benzene ring on the left.
2. Place another one on the right.
3. Add a single bond to the top of the right ring.

Step 2: Compare them

1. Open the [full editor](#) in a new tab.
2. Sign in. Install **Compare Molecules** from **Settings, Plugins**.
3. Draw benzene. Open the **Compare** tab. Click **Add canvas**.
4. Type **Cc1ccccc1 toluene** in the SMILES box. Click **Add SMILES**.
5. Come back and click

Try it in the editor

Chapter complete

Next: How to look up a molecule in ChEMBL

[Next chapter](#)

The full MolDraw editor opens here. It loads when you open this tab.

Questions and answers

What is a Tanimoto score?

A number from 0 to 1. A score of 1 means the fingerprints are the same.

Can I compare many molecules?

Yes. Add one SMILES per line.

For more detail, read [the guide in the docs](#).

How to turn a name or SMILES into a structure | Learn MolDraw

<https://www.moldraw.com/learn/how-to-convert-a-name-or-smiles-to-a-structure/>

Click Paste SMILES and type a SMILES string, or type a name in the PubChem search box. MolDraw draws the structure for you.

Beginner 4 min 3 steps

Short answer: Click Paste SMILES and type a SMILES string, or type a name in the PubChem search box. MolDraw draws the structure for you.

You will learn to: Paste a SMILES string; Search a name in PubChem; Copy SMILES from your drawing.

1 Watch demo 2 Try in editor

Watch the demo

From text to structure in about 20 seconds.

The steps in text

Step 1: Paste the SMILES of caffeine

1. Click [here](#).
2. Click **Paste SMILES** in the editor. If a box opens, press Ctrl+V and Enter. Then press Esc.

Step 2: Search aspirin by name

1. Click **Clear canvas**.
2. Click the **PubChem** search box at the top. Type **aspirin** and press Enter.

Step 3: Copy the SMILES

1. Click **Copy SMILES** in the top row.

Try it in the editor

Chapter complete

Next: How to find the formula, weight and IUPAC name

[Next chapter](#)

The full MolDraw editor opens here. It loads when you open this tab.

Questions and answers

Can I paste a SMILES string?

Yes. Click Paste SMILES in the editor and type or paste the text.

Can I search by name?

Yes. Type a name or CAS number in the PubChem box at the top.

How do I copy SMILES?

Click Copy SMILES in the top row.

For more detail, read [the guide in the docs](#).

How to draw a reaction scheme with arrows | Learn MolDraw

<https://www.moldraw.com/learn/how-to-draw-a-chemical-reaction-scheme-with-arrows/>

Draw the starting material, add a reaction arrow, draw the product, then type the reagents above the arrow.

Beginner 6 min 4 steps

Short answer: Draw the starting material, add a reaction arrow, draw the product, then type the reagents above the arrow.

You will learn to: Draw a reactant; Add a reaction arrow; Draw the product; Type reagents on the scheme.

1 Watch demo 2 Try in editor

Watch the demo

A reaction scheme in about 25 seconds.

The steps in text

Step 1: Draw ethene on the left

1. Draw one bond on the left side of the canvas.
2. Make it a double bond with the bond menu or 2.

Step 2: Add a reaction arrow

1. Pick the **reaction arrow** tool in the left rail.
2. Drag from right of ethene toward the right.

Step 3: Draw ethane on the right

1. Pick **Single** in the bond menu.
2. Click an empty spot to the right of the arrow.

Step 4: Type the reagents

1. Pick the **Text** tool (the T in the tools row).
2. Click just above the arrow. Type **H₂, Pd**. Press Esc.

Try it in the editor

Chapter complete

Next: How to draw curved arrow mechanisms

[Next chapter](#)

The full MolDraw editor opens here. It loads when you open this tab.

Questions and answers

How do I add reagents to an arrow?

Use the Text tool and type above or below the arrow.

Can I draw equilibrium arrows?

Yes. Open the arrow menu and pick Equilibrium.

Can I copy a reaction as SMILES?

Yes. Copy SMILES gives reaction SMILES like A>>B when an arrow is on the canvas.

For more detail, read [the guide in the docs](#).

How to draw a benzene ring and phenol | Learn MolDraw

<https://www.moldraw.com/learn/how-to-draw-benzene-ring-and-phenol-structure/>

Draw a benzene ring, then add an OH group to make phenol. The editor checks each step as you draw.

Beginner 5 min 2 steps

Short answer: Draw a benzene ring, then add an OH group to make phenol. The editor checks each step as you draw.

You will learn to: Place a ring from the ring bar; Add a bond to a ring atom; Change an atom to oxygen.

1 Watch demo 2 Try in editor

Watch the demo

Watch this first. It takes about 20 seconds.

The steps in text

Step 1: Draw benzene

1. Click the benzene button in the ring bar at the bottom left.
2. Click an empty spot on the canvas.

Step 2: Turn it into phenol

1. Click the single bond tool in the left rail.
2. Click the top atom of the ring. A new bond appears.
3. Click **O** in the atom palette. Then click the end of the new bond.

Try it in the editor

Chapter complete

Next: How to draw double, triple and wedge bonds

[Next chapter](#)

The full MolDraw editor opens here. It loads when you open this tab.

Questions and answers

What is phenol?

Phenol is benzene with one OH group. Its formula is C₆H₆O.

How does the check work?

The editor sends your drawing to the page each time you change it. The page compares every atom, bond and charge with the answer. Position and size do not matter.

Is my progress saved?

Yes. It saves in this browser.

For more detail, read [the guide in the docs](#).

How to draw double, triple and wedge bonds | Learn MolDraw

<https://www.moldraw.com/learn/how-to-draw-chemical-bonds-double-triple-and-wedge-bonds/>

Pick a bond type from the bond menu, then click a bond to change it. Press 1, 2 or 3 for single, double or triple bonds.

Beginner 5 min 3 steps

Short answer: Pick a bond type from the bond menu, then click a bond to change it. Press 1, 2 or 3 for single, double or triple bonds.

You will learn to: Draw a single bond; Change it to a double and a triple bond; Add a wedge bond.

1 Watch demo 2 Try in editor

Watch the demo

Bond types in about 20 seconds.

The steps in text

Step 1: Draw ethene

1. Click the single bond tool in the left rail. Then click an empty spot. You get one bond.
2. Open the bond menu with the small arrow next to the bond tool. Pick **Double**. You can also press 2.
3. Click the middle of your bond.

Step 2: Make it ethyne

1. Pick **Triple** in the bond menu, or press 3.
2. Click the middle of the double bond.

Step 3: Add a wedge bond

1. Pick **Wedge up** in the bond menu.
2. Click the left atom. A wedge bond grows from it.

Try it in the editor

Chapter complete

Next: How to add atoms, elements and formal charges

[Next chapter](#)

The full MolDraw editor opens here. It loads when you open this tab.

Questions and answers

How do I draw a double bond?

Pick Double in the bond menu, or press 2. Then click a bond.

How do I draw a triple bond?

Pick Triple in the bond menu, or press 3. Then click a bond.

What does a wedge bond mean?

A wedge bond points toward you. A hashed bond points away from you.

For more detail, read [the guide in the docs](#).

How to draw curved arrow mechanisms | Learn MolDraw

<https://www.moldraw.com/learn/how-to-draw-curved-arrow-reaction-mechanisms/>

Draw the species, add lone pairs, then draw a curved arrow from the electrons to the atom that receives them.

Beginner 6 min 4 steps

Short answer: Draw the species, add lone pairs, then draw a curved arrow from the electrons to the atom that receives them.

You will learn to: Draw hydroxide and chloromethane; Show lone pairs on oxygen; Draw a curved arrow.

1 Watch demo 2 Try in editor

Watch the demo

A mechanism step in about 25 seconds.

The steps in text

Step 1: Draw hydroxide

1. Click **O** in the atom palette and click the left side of the canvas.
2. Pick the **minus** tool in the left rail. Click the O.

Step 2: Draw chloromethane

1. Click **C** in the palette. Pick the single bond tool. Click to the right of hydroxide.
2. Click **Cl** in the atom palette. Click the right end of the new bond.

Step 3: Add lone pairs to O

1. Pick the **lone pair** tool.
2. Click the O atom two times.

Step 4: Draw a curved arrow

1. Open the arrow menu (small arrow next to the reaction arrow tool). Pick **Curved**.
2. Drag from the O toward the carbon.

Try it in the editor

Chapter complete

Next: How to turn a name or SMILES into a structure

[Next chapter](#)

The full MolDraw editor opens here. It loads when you open this tab.

Questions and answers

Where should a curved arrow start?

Start it at a lone pair or a bond. Electrons move from there.

What is a fishhook arrow?

A fishhook arrow moves one electron. Use it for radical steps.

Can I bend a curved arrow?

Yes. Drag its middle handle to change the curve.

For more detail, read [the guide in the docs](#).

How to draw lab apparatus and glassware | Learn MolDraw

<https://www.moldraw.com/learn/how-to-draw-lab-apparatus-and-glassware/>

Open the Draw tab, pick Glassware and drag a flask onto the canvas. Then label it.

Beginner 3 min 2 steps

Short answer: Open the Draw tab, pick Glassware and drag a flask onto the canvas. Then label it.

You will learn to: Find the Glassware tool; Place a flask; Label it with text.

1 Watch demo2 Try in editor

Watch the demo

Glassware in about 15 seconds.

The steps in text

Step 1: Place a flask

1. Click the **Draw** tab at the top.
2. Pick **Glassware** (the flask icon).
3. Drag on the canvas.

Step 2: Label the flask

1. Click the **Home** tab. Pick the **Text** tool.
2. Click beside the flask. Type **Reaction flask**. Press Esc.

Try it in the editor

Chapter complete

Next: How to add ligands and functional groups

[Next chapter](#)

The full MolDraw editor opens here. It loads when you open this tab.

Questions and answers

What are Sciicons?

Sciicons is a library of science icons. Open it from the Glassware menu in the Draw tab.

Can I fill the flask with liquid?

Yes. Select the flask and change its liquid fill.

For more detail, read [the guide in the docs](#).

How to draw lone pairs and radicals | Learn MolDraw

<https://www.moldraw.com/learn/how-to-draw-lone-pairs-and-radicals-on-atoms/>

Pick the lone pair tool and click an atom to add a pair of dots. Pick Free radical in the same menu to add a single dot.

Beginner 4 min 3 steps

Short answer: Pick the lone pair tool and click an atom to add a pair of dots. Pick Free radical in the same menu to add a single dot.

You will learn to: Place a single atom; Add two lone pairs to oxygen; Add a radical dot.

1 Watch demo 2 Try in editor

Watch the demo

Lone pairs and radicals in about 15 seconds.

The steps in text

Step 1: Draw water

1. Click **O** in the atom palette.
2. Click an empty spot on the canvas. You get H₂O.

Step 2: Add two lone pairs to O

1. Pick the **lone pair** tool in the left rail. It shows two dots.
2. Click the O atom twice.

Step 3: Draw a methyl radical

1. Click **Clear canvas** (the red bin).
2. Click **C** in the atom palette. Click an empty spot.
3. Open the lone pair menu (small arrow) and pick **Free radical**. Click the C atom.

Try it in the editor

Chapter complete

Next: How to draw rings, chairs and fused rings

[Next chapter](#)

The full MolDraw editor opens here. It loads when you open this tab.

Questions and answers

How many lone pairs does water have?

The oxygen in water has two lone pairs.

How do I draw a radical?

Open the lone pair menu, pick Free radical, then click the atom.

Can I move lone pairs?

Yes. Drag the dots around the atom with the select tool.

For more detail, read [the guide in the docs](#).

How to draw polymer repeat unit brackets | Learn MolDraw

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

Draw one ethylene unit, then drag polymer brackets around it to show polyethylene.

Beginner 3 min 2 steps

Short answer: Draw one ethylene unit, then drag polymer brackets around it to show polyethylene.

You will learn to: Draw a C-C bond; Add polymer brackets with n.

1 Watch demo 2 Try in editor

Watch the demo

Brackets in about 15 seconds.

The steps in text

Step 1: Draw the repeat unit

1. Pick the single bond tool. Click an empty spot.

Step 2: Add the brackets

1. Click the [] brackets tool in the left rail.
2. Drag a box over the bond.

Try it in the editor

Chapter complete

Next: How to add text and shapes to a drawing

[Next chapter](#)

The full MolDraw editor opens here. It loads when you open this tab.

Questions and answers

How do I change n?

Click the subscript under the right bracket and type a new value.

Can I draw copolymers?

Yes. Click the brackets tool again to pick copolymer or parenthesis.

For more detail, read [the guide in the docs](#).

How to draw rings, chairs and fused rings | Learn MolDraw

<https://www.moldraw.com/learn/how-to-draw-rings-cyclohexane-chair-and-fused-rings/>

Pick a ring in the ring bar and click the canvas. Click a ring bond with benzene to fuse a second ring. Pick Chair to draw a cyclohexane chair.

Beginner 5 min 3 steps

Short answer: Pick a ring in the ring bar and click the canvas. Click a ring bond with benzene to fuse a second ring. Pick Chair to draw a cyclohexane chair.

You will learn to: Place a cyclohexane ring; Fuse two rings into naphthalene; Draw a cyclohexane chair.

1 Watch demo 2 Try in editor

Watch the demo

Rings in about 20 seconds.

The steps in text

Step 1: Draw cyclohexane

1. Open the menu on the **C6** ring button (small arrow) and pick **Flat C6**.
2. Click an empty spot.

Step 2: Draw naphthalene

1. Click **Clear canvas**.
2. Pick benzene and click the canvas.
3. Keep benzene picked. Click the right side bond of the ring.

Step 3: Draw a cyclohexane chair

1. Click **Clear canvas**.
2. Open the C6 ring menu and pick **Chair**.
3. Click an empty spot.

Try it in the editor

Chapter complete

Next: How to use R groups and labels like Ph and COOH

[Next chapter](#)

The full MolDraw editor opens here. It loads when you open this tab.

Questions and answers

How do I draw naphthalene?

Place benzene, then click one of its bonds with the benzene tool.

How do I draw a chair conformation?

Open the C6 ring menu, pick Chair and click the canvas.

Which ring sizes can I draw?

The ring bar has rings from 3 to 8 atoms.

For more detail, read [the guide in the docs](#).

How to draw stereochemistry with wedge and hash bonds | Learn MolDraw

<https://www.moldraw.com/learn/how-to-draw-stereochemistry-with-wedge-and-hash-bonds/>

Change a bond at a stereocenter to a wedge or hash bond. Turn on R and S labels in Settings to see the configuration.

Beginner 5 min 3 steps

Short answer: Change a bond at a stereocenter to a wedge or hash bond. Turn on R and S labels in Settings to see the configuration.

You will learn to: Load a structure from SMILES; Make a wedge bond at a stereocenter; Show R and S labels.

1 Watch demo 2 Try in editor

Watch the demo

Stereochemistry in about 20 seconds.

The steps in text

Step 1: Load butan-2-ol

1. Click [here](#).
2. Click **Paste SMILES** in the editor. If a box opens, press Ctrl+V and Enter. Then press Esc.

Step 2: Make the C to O bond a wedge

1. Pick **Wedge up** in the bond menu.
2. Click the middle of the bond between the stereocenter and O.

Step 3: Show R and S labels

1. Click **Settings** (the gear) in the tools row.
2. Turn on **R/S and E/Z labels**. Close Settings.

Try it in the editor

Chapter complete

Next: How to draw a reaction scheme with arrows

[Next chapter](#)

The full MolDraw editor opens here. It loads when you open this tab.

Questions and answers

How do I show R and S labels?

Open Settings and turn on R/S and E/Z labels.

What is the difference between wedge and hash bonds?

A wedge points toward you. A hash points away from you.

Does MolDraw keep stereo in SMILES?

Yes. Copy SMILES includes @ and @@ for drawn stereocenters.

For more detail, read [the guide in the docs](#).

How to export a structure for a paper or slides | Learn MolDraw

<https://www.moldraw.com/learn/how-to-export-a-chemical-structure-for-a-paper-or-slides/>

Click Download and pick SVG or PDF for papers, or PNG for slides.

Beginner 4 min 3 steps

Short answer: Click Download and pick SVG or PDF for papers, or PNG for slides.

You will learn to: Draw a structure; Download an SVG; Download a PNG.

1 Watch demo 2 Try in editor

Watch the demo

Export in about 15 seconds.

The steps in text

Step 1: Draw benzene

1. Pick benzene in the ring bar and click the canvas.

Step 2: Download an SVG

1. Click **Download** in the top row.
2. Click **SVG**.

Step 3: Download a PNG

1. Click **Download** again.
2. Click **PNG**. Pick a size, then click **Export**.

Try it in the editor

Chapter complete

Next: How to predict an NMR spectrum from a structure

[Next chapter](#)

The full MolDraw editor opens here. It loads when you open this tab.

Questions and answers

Which format is best for a paper?

Use SVG or PDF. They stay sharp at any size.

Which format is best for slides?

Use PNG or SVG. Both paste well into PowerPoint and Google Slides.

Can I export a transparent PNG?

Yes. Pick PNG. Pick PNG white for a white background.

For more detail, read [the guide in the docs](#).

How to export MOL, SVG and other file formats | Learn MolDraw

<https://www.moldraw.com/learn/how-to-export-mol-svg-and-other-chemical-file-formats/>

Draw benzene, then download it as a MOL file and as an SVG image.

Beginner 3 min 3 steps

Short answer: Draw benzene, then download it as a MOL file and as an SVG image.

You will learn to: Download a MOL file; Download an SVG image.

1 Watch demo2 Try in editor

Watch the demo

File formats in about 15 seconds.

The steps in text

Step 1: Draw benzene

1. Click the benzene button in the ring bar. Click the canvas.

Step 2: Download a MOL file

1. Click **Download** at the right of the top row.
2. Click **MOL**.

Step 3: Download an SVG

1. Click **Download** again.
2. Click **SVG**.

Try it in the editor

Chapter complete

Next: How to open the AI chemistry assistant

[Next chapter](#)

The full MolDraw editor opens here. It loads when you open this tab.

Questions and answers

Which format should I use?

Use MOL or SDF to share structures. Use SVG or PNG for images. Use CDXML for ChemDraw.

Can I open files too?

Yes. Use File, Open for MOL, CDX, CDXML and MolDraw files.

For more detail, read [the guide in the docs](#).

How to find the formula, weight and IUPAC name | Learn MolDraw

<https://www.moldraw.com/learn/how-to-find-molecular-formula-weight-and-iupac-name/>

Select your molecule and click Info. The panel shows the name, formula and weight. Click Copy IUPAC to copy the name.

Beginner 4 min 3 steps

Short answer: Select your molecule and click Info. The panel shows the name, formula and weight. Click Copy IUPAC to copy the name.

You will learn to: Draw a molecule; Open the Info panel; Copy the IUPAC name.

1 Watch demo 2 Try in editor

Watch the demo

Molecule info in about 15 seconds.

The steps in text

Step 1: Draw ethanol

1. Draw one bond. Change the left atom to **O**.
2. Click **C** in the palette. Then click the right atom with the bond tool to add a carbon.

Step 2: Open the Info panel

1. Press Ctrl+A to select all.
2. Click **Info** at the top.

Step 3: Copy the IUPAC name

1. In the Info panel, click **Copy IUPAC**.

Try it in the editor

Chapter complete

Next: How to view a molecule in 3D

[Next chapter](#)

The full MolDraw editor opens here. It loads when you open this tab.

Questions and answers

How do I get the IUPAC name?

Select the molecule and click Info. Then click Copy IUPAC.

Does the weight include hydrogens?

Yes. The formula and weight count all implied hydrogens.

Can I see logP and exact mass?

Yes. They are in the same Info panel.

For more detail, read [the guide in the docs](#).

How to look up a molecule in ChEMBL | Learn MolDraw

<https://www.moldraw.com/learn/how-to-look-up-a-molecule-in-chembl/>

Load aspirin here, then find its targets and activity data with the ChEMBL plugin.

Beginner 4 min 2 steps

Short answer: Load aspirin here, then find its targets and activity data with the ChEMBL plugin.

You will learn to: Load aspirin; Search ChEMBL; Read targets and activity.

1 Watch demo 2 Try in editor

Watch the demo

The molecule for this chapter, in about 10 seconds.

The steps in text

Step 1: Load aspirin

1. Click the **PubChem** search box. Type **aspirin**. Press Enter.

Step 2: Search ChEMBL

1. Open the [full editor](#) in a new tab.
2. Sign in. Install **ChEMBL** from **Settings, Plugins**.
3. Open the **ChEMBL** tab. Type **CHEMBL25**. Click **Lookup**.
4. Open the **Targets** and **Activity** tabs.
5. Come back and click

Try it in the editor

Chapter complete

Next: How to view a protein structure from the PDB

[Next chapter](#)

The full MolDraw editor opens here. It loads when you open this tab.

Questions and answers

What is ChEMBL?

A free database of drug-like molecules and their bioactivity.

What is ChEMBL25?

It is the ChEMBL ID for aspirin.

For more detail, read [the guide in the docs](#).

How to make publication quality structure figures | Learn MolDraw

<https://www.moldraw.com/learn/how-to-make-publication-quality-chemical-structure-figures/>

Pick the ACS Document 1996 style in Settings, Style presets. Then download a PDF or SVG for your paper.

Beginner 5 min 3 steps

Short answer: Pick the ACS Document 1996 style in Settings, Style presets. Then download a PDF or SVG for your paper.

You will learn to: Draw a structure; Apply the ACS 1996 style; Export a PDF.

1 Watch demo 2 Try in editor

Watch the demo

A journal figure in about 25 seconds.

The steps in text

Step 1: Load aspirin

1. Click [here](#).
2. Click **Paste SMILES** in the editor. If a box opens, press Ctrl+V and Enter. Then press Esc.

Step 2: Apply ACS 1996 style

1. Click **Settings**. Open **Style presets**.
2. Click **ACS Document 1996**. Close Settings.

Step 3: Download a PDF

1. Click **Download**.
2. Click **PDF**.

Try it in the editor

Chapter complete

Next: How to clean up a chemical structure

[Next chapter](#)

The full MolDraw editor opens here. It loads when you open this tab.

Questions and answers

What is ACS 1996 style?

It is a common journal style for chemical drawings. It fixes bond length, line width and font.

Which file type is best for journals?

Use PDF, SVG or EPS. They stay sharp at any size.

Can I also send a CDXML file?

Yes. Download CDXML if the journal asks for ChemDraw files.

For more detail, read [the guide in the docs](#).

How to map atoms in a reaction | Learn MolDraw

<https://www.moldraw.com/learn/how-to-map-atoms-in-a-reaction/>

Draw a simple reaction here, then number matching atoms with Automap in the full editor.

Beginner 4 min 2 steps

Short answer: Draw a simple reaction here, then number matching atoms with Automap in the full editor.

You will learn to: Draw a reaction with an arrow; Run Automap.

1 Watch demo 2 Try in editor

Watch the demo

A reaction in about 15 seconds.

The steps in text

Step 1: Draw ethene to ethane

1. Draw ethene: one bond, then make it double with **Double** from the bond menu.
2. Pick the reaction arrow tool. Drag to the right of ethene.
3. Draw a single bond right of the arrow.

Step 2: Run Automap

1. Open the [full editor](#) in a new tab.
2. Draw the same reaction.
3. Open the **Chemistry** menu. Click **Automap**.
4. Each atom now shows a number. The same number marks the same atom on both sides.
5. Come back and click

Try it in the editor

Chapter complete

Next: How to use Community, Dashboard and your profile

[Next chapter](#)

The full MolDraw editor opens here. It loads when you open this tab.

Questions and answers

What is atom mapping?

It numbers each reactant atom and the product atom it becomes.

Why map atoms?

Maps help track bonds that form and break. Reaction databases use them.

For more detail, read [the guide in the docs](#).

How to open the AI chemistry assistant | Learn MolDraw

<https://www.moldraw.com/learn/how-to-open-the-ai-chemistry-assistant/>

Open AI chat from the tools row. Ask it to draw a molecule from a name or a description.

Beginner 2 min 2 steps

Short answer: Open AI chat from the tools row. Ask it to draw a molecule from a name or a description.

You will learn to: Open AI chat; Know what to ask it.

1 Watch demo 2 Try in editor

Watch the demo

AI chat in about 10 seconds.

The steps in text

Step 1: Draw benzene

1. Click the benzene button in the ring bar. Click the canvas.

Step 2: Open AI chat

1. Open the [full editor](#) in a new tab. AI chat is not in this practice editor.
2. Click **AI chat** in the tools row (the sparkle icon).
3. Ask: *Draw nitrobenzene.*
4. Come back and click

Try it in the editor

Chapter complete

Next: How to sketch structures with Smart Draw

[Next chapter](#)

The full MolDraw editor opens here. It loads when you open this tab.

Questions and answers

What can the AI do?

It can draw a structure from a name or a description, edit your drawing and explain it.

Is it free?

You can use it with a free account, or add your own Gemini key in Settings.

For more detail, read [the guide in the docs](#).

How to predict a mass spectrum | Learn MolDraw

<https://www.moldraw.com/learn/how-to-predict-a-mass-spectrum/>

Draw ethanol here, then ask the AI Spectroscopy plugin for its mass spectrum in the full editor.

Beginner 4 min 2 steps

Short answer: Draw ethanol here, then ask the AI Spectroscopy plugin for its mass spectrum in the full editor.

You will learn to: Draw ethanol; Install AI Spectroscopy; Ask for a mass spectrum.

1 Watch demo 2 Try in editor

Watch the demo

The molecule for this chapter, in about 10 seconds.

The steps in text

Step 1: Draw ethanol

1. Pick the single bond tool. Click the canvas.
2. Pick **O** in the atom palette. Click the right end.
3. Pick **C**, then the bond tool. Click the left end.

Step 2: Predict its mass spectrum

1. Open the [full editor](#) in a new tab.
2. Sign in. Install **AI Spectroscopy** from **Settings, Plugins**.
3. Add your Gemini key in **Settings, AI**.
4. Draw ethanol. Click **AI chat**. Type *Predict the mass spectrum*.
5. Come back and click

Try it in the editor

Chapter complete

Next: How to show an electrostatic potential map

[Next chapter](#)

The full MolDraw editor opens here. It loads when you open this tab.

Questions and answers

What is the molecular ion?

It is the peak at the mass of the whole molecule. For ethanol it is m/z 46.

Is the prediction exact?

No. It is an estimate. Check it against measured data.

For more detail, read [the guide in the docs](#).

How to predict an NMR spectrum from a structure | Learn MolDraw

<https://www.moldraw.com/learn/how-to-predict-an-nmr-spectrum-from-a-structure/>

Draw the molecule and copy its SMILES. Paste it into the free MolDraw NMR predictor, or use the NMR Analyser plugin with a free account.

Beginner 4 min 2 steps

Short answer: Draw the molecule and copy its SMILES. Paste it into the free MolDraw NMR predictor, or use the NMR Analyser plugin with a free account.

You will learn to: Draw ethanol; Copy its SMILES; Open the NMR predictor.

1 Watch demo 2 Try in editor

Watch the demo

Ready for NMR in about 15 seconds.

The steps in text

Step 1: Draw ethanol

1. Draw one bond. Change the left atom to **O**.
2. Click **C** in the palette. Then click the right atom with the bond tool.

Step 2: Copy the SMILES

1. Click **Copy SMILES** in the top row.
2. Open the [free NMR predictor](#) in a new tab and paste it.

Try it in the editor

Chapter complete

Next: How to change atom colours and colour a structure

[Next chapter](#)

The full MolDraw editor opens here. It loads when you open this tab.

Questions and answers

Is NMR prediction free?

Yes. The online predictor is free. The NMR Analyser plugin is free with an account.

Which spectra can I predict?

You can predict ^1H and ^{13}C NMR. The plugin also shows 2D spectra.

How many peaks does ethanol show in ^1H NMR?

Three: CH_3 , CH_2 and OH .

For more detail, read [the guide in the docs](#).

How to search PubChem by name or CAS number | Learn

MolDraw

<https://www.moldraw.com/learn/how-to-search-pubchem-by-name-or-cas-number/>

Type a name or a CAS number in the PubChem box. MolDraw draws the structure for you.

Beginner 3 min 2 steps

Short answer: Type a name or a CAS number in the PubChem box. MolDraw draws the structure for you.

You will learn to: Search by name; Search by CAS number.

1 Watch demo 2 Try in editor

Watch the demo

PubChem search in about 20 seconds.

The steps in text

Step 1: Search by name

1. Click the **PubChem** search box at the top.
2. Type **caffeine**. Press Enter.

Step 2: Search by CAS number

1. Click **Clear canvas** (the red bin).
2. Type **50-78-2** in the PubChem box. Press Enter.

Try it in the editor

Chapter complete

Next: How to export MOL, SVG and other file formats

[Next chapter](#)

The full MolDraw editor opens here. It loads when you open this tab.

Questions and answers

What is a CAS number?

A unique ID for a chemical, such as 50-78-2 for aspirin.

Does search work offline?

No. PubChem search needs the internet.

For more detail, read [the guide in the docs](#).

How to set bond length, line width and bond style | Learn MolDraw

<https://www.moldraw.com/learn/how-to-set-bond-length-line-width-and-bond-style/>

Open Color and style, then Bonds. Set Bond thickness for line width and Bond length for size.

Beginner 4 min 3 steps

Short answer: Open Color and style, then Bonds. Set Bond thickness for line width and Bond length for size.

You will learn to: Open the Bonds style section; Make bonds thicker; Make bonds longer.

1 Watch demo 2 Try in editor

Watch the demo

Bond style in about 15 seconds.

The steps in text

Step 1: Draw benzene

1. Pick benzene in the ring bar and click the canvas.

Step 2: Set bond thickness to 3 px

1. Click **Color and style**. Open **Bonds**.
2. Set **Bond thickness** to **3 px**.

Step 3: Set bond length to 60 px

1. In the same section, set **Bond length** to **60 px**.

Try it in the editor

Chapter complete

Next: How to use themes and ball and stick style

[Next chapter](#)

The full MolDraw editor opens here. It loads when you open this tab.

Questions and answers

How do I make bonds thicker?

Open Color and style, then Bonds, and raise Bond thickness.

What bond length do journals use?

Many journals use the ACS 1996 style. Pick it in Settings, Style presets.

Can I change the double bond gap?

Yes. Set Double bond gap in the same Bonds section.

For more detail, read [the guide in the docs](#).

How to show an electrostatic potential map | Learn MolDraw

<https://www.moldraw.com/learn/how-to-show-an-electrostatic-potential-map/>

Draw phenol here, then colour its 3D surface by charge with the MEP plugin.

Beginner 4 min 2 steps

Short answer: Draw phenol here, then colour its 3D surface by charge with the MEP plugin.

You will learn to: Draw phenol; Open the MEP tab; Read the colour scale.

1 Watch demo 2 Try in editor

Watch the demo

The molecule for this chapter, in about 15 seconds.

The steps in text

Step 1: Draw phenol

1. Place benzene from the ring bar.
2. Pick the single bond tool. Click the top ring atom.
3. Pick **O**. Click the end of the new bond.

Step 2: Show the MEP surface

1. Open the [full editor](#) in a new tab.
2. Sign in. Install **Electrostatic Potential (MEP)** from **Settings, Plugins**.
3. Draw phenol. Open the **MEP** tab.
4. Click **Show in 3D**.
5. Come back and click

Try it in the editor

Chapter complete

Next: How to compare two molecules for similarity

[Next chapter](#)

The full MolDraw editor opens here. It loads when you open this tab.

Questions and answers

How are the charges calculated?

MolDraw uses Gasteiger partial charges.

What do the colours mean?

Red is electron-rich. Blue is electron-poor.

For more detail, read [the guide in the docs](#).

How to use Community, Dashboard and your profile | Learn MolDraw

<https://www.moldraw.com/learn/how-to-use-community-dashboard-and-profile/>

Sign in to save designs online, share them in Community and manage them from your Dashboard.

Beginner 3 min 2 steps

Short answer: Sign in to save designs online, share them in Community and manage them from your Dashboard.

You will learn to: Sign in; Find My designs and Dashboard; Visit Community.

1 Watch demo 2 Try in editor

Watch the demo

The design to save, in about 5 seconds.

The steps in text

Step 1: Draw benzene

1. Click the benzene button in the ring bar. Click the canvas.

Step 2: Explore your account

1. Open the [full editor](#) in a new tab.
2. Click **Sign in**. Use Google or email.
3. Fill in your profile when asked.
4. Click **My designs** to see saved work. Open **Dashboard** from your avatar.
5. Click **Community** to see shared posts and feature requests.
6. Come back and click

Try it in the editor

Chapter complete

Next: All chapters

[Next chapter](#)

The full MolDraw editor opens here. It loads when you open this tab.

Questions and answers

Do I need an account?

No for drawing. Yes for plugins, cloud saving and Community posts.

Where is my work saved?

Without an account, in this browser. With an account, online too.

For more detail, read [the guide in the docs](#).

How to use keyboard shortcuts to draw faster | Learn MolDraw

<https://www.moldraw.com/learn/how-to-use-keyboard-shortcuts-to-draw-faster/>

Use Ctrl+A, Delete and Ctrl+Z to select, clear and undo in seconds.

Beginner 3 min 3 steps

Short answer: Use Ctrl+A, Delete and Ctrl+Z to select, clear and undo in seconds.

You will learn to: Select all with Ctrl+A; Delete with the Delete key; Undo with Ctrl+Z.

1 Watch demo 2 Try in editor

Watch the demo

Shortcuts in about 15 seconds.

The steps in text

Step 1: Draw benzene

1. Click the benzene button in the ring bar. Click the canvas.

Step 2: Select all and delete

1. Pick the **Hand** tool at the top of the left rail. Click an empty spot.
2. Press Ctrl+A. Then press Delete.

Step 3: Undo it

1. Press Ctrl+Z.

Try it in the editor

Chapter complete

Next: How to draw lab apparatus and glassware

[Next chapter](#)

The full MolDraw editor opens here. It loads when you open this tab.

Questions and answers

Where is the full list?

See the keyboard shortcuts page in the docs. You can remap keys in Settings, Shortcuts.

Which keys draw atoms?

Press C, N, O, S and other element keys with the atom tool.

For more detail, read [the guide in the docs](#).

How to use R groups and labels like Ph and COOH | Learn MolDraw

<https://www.moldraw.com/learn/how-to-use-r-groups-and-atom-labels-like-ph-and-cooh/>

Pick the atom label tool, click an atom and type a label such as Ph, COOH or R1. Press Enter to finish.

Beginner 4 min 3 steps

Short answer: Pick the atom label tool, click an atom and type a label such as Ph, COOH or R1. Press Enter to finish.

You will learn to: Type a short label on an atom; Add a COOH group label; Mark an R group.

1 Watch demo 2 Try in editor

Watch the demo

Labels in about 20 seconds.

The steps in text

Step 1: Label an atom Ph

1. Draw one bond with the single bond tool.

2. Pick the **A** atom label tool in the left rail.
3. Click the left atom. Type **Ph** and press Enter.

Step 2: Label the other end COOH

1. Keep the label tool picked.
2. Click the right atom. Type **COOH** and press Enter.

Step 3: Add an R group

1. Draw a new bond below the first one.
2. With the label tool, click its left atom. Type **R1** and press Enter.

Try it in the editor

Chapter complete

Next: How to draw stereochemistry with wedge and hash bonds

[Next chapter](#)

The full MolDraw editor opens here. It loads when you open this tab.

Questions and answers

How do I add an R group?

Use the atom label tool and type R1 on an atom.

Can MolDraw expand a label like Ph?

Yes. Right click the label and pick expand to see all atoms.

Which labels does MolDraw know?

It knows common groups like Me, Et, Ph, Boc, OMe, NH₂ and COOH.

For more detail, read [the guide in the docs](#).

How to use ring templates and the structure library | Learn MolDraw

<https://www.moldraw.com/learn/how-to-use-ring-templates-and-the-structure-library/>

Place a ring from the ring bar, then add a ready-made amino acid from the Library.

Beginner 4 min 2 steps

Short answer: Place a ring from the ring bar, then add a ready-made amino acid from the Library.

You will learn to: Place a cyclopentane ring; Open the Library; Add glycine to the canvas.

1 Watch demo2 Try in editor

Watch the demo

Templates in about 20 seconds.

The steps in text

Step 1: Place cyclopentane

1. Click the pentagon in the ring bar at the bottom.
2. Click an empty spot.

Step 2: Add glycine from the Library

1. Click **Library** at the right end of the ring bar.
2. Click **Glycine**.
3. Click an empty spot on the canvas.

Try it in the editor

Chapter complete

Next: How to draw polymer repeat unit brackets

[Next chapter](#)

The full MolDraw editor opens here. It loads when you open this tab.

Questions and answers

What is in the Library?

Rings, R-groups, ligands, sugars, amino acids, polymers, MOFs and named reactions.

Can I drag from the Library?

Yes. Click or drag a card onto the canvas.

For more detail, read [the guide in the docs](#).

How to sketch structures with Smart Draw | Learn MolDraw

<https://www.moldraw.com/learn/how-to-use-smart-draw-to-sketch-structures/>

Smart Draw turns freehand strokes into bonds, rings and labels. Draw cyclohexane here, then sketch it in the full editor.

Beginner 4 min 2 steps

Short answer: Smart Draw turns freehand strokes into bonds, rings and labels. Draw cyclohexane here, then sketch it in the full editor.

You will learn to: Know what Smart Draw recognises; Install the Smart Draw plugin; Sketch a ring.

1 Watch demo2 Try in editor

Watch the demo

The ring you will sketch, in about 10 seconds.

The steps in text

Step 1: Place cyclohexane

1. Click the plain hexagon in the ring bar. Click the canvas.

Step 2: Sketch it with Smart Draw

1. Open the [full editor](#) in a new tab.
2. Sign in. Click **Settings**, **Plugins**, then **Install** next to Smart Draw.
3. Pick **Smart Draw** in the left toolbar.
4. Sketch a closed six-sided shape. It becomes a ring.
5. Come back and click

Try it in the editor

Chapter complete

Next: How to predict a mass spectrum

[Next chapter](#)

The full MolDraw editor opens here. It loads when you open this tab.

Questions and answers

What does Smart Draw recognise?

Straight strokes become bonds. Closed shapes become rings. Written letters become atom labels.

Do I need an account?

Yes. Plugins install after you sign in.

For more detail, read [the guide in the docs](#).

How to use themes and ball and stick style | Learn MolDraw

<https://www.moldraw.com/learn/how-to-use-themes-and-ball-and-stick-style-for-molecules/>

Open Color and style and set Look to Ball and stick. Set it back to Default for the plain line style.

Beginner 3 min 3 steps

Short answer: Open Color and style and set Look to Ball and stick. Set it back to Default for the plain line style.

You will learn to: Draw a molecule; Switch to ball and stick; Go back to the default look.

1 Watch demo 2 Try in editor

Watch the demo

Themes in about 15 seconds.

The steps in text

Step 1: Draw benzene

1. Pick benzene in the ring bar and click the canvas.

Step 2: Switch to ball and stick

1. Click **Color and style**.
2. Set **Look** to **Ball and stick**.

Step 3: Go back to the default look

1. Set **Look** back to **Default**.

Try it in the editor

Chapter complete

Next: How to align, arrange and space out structures

[Next chapter](#)

The full MolDraw editor opens here. It loads when you open this tab.

Questions and answers

How do I draw ball and stick in 2D?

Open Color and style and set Look to Ball and stick.

Does the look change my file?

No. It only changes how the drawing looks. The structure stays the same.

Can I export ball and stick images?

Yes. PNG, SVG and PDF use the look you pick.

For more detail, read [the guide in the docs](#).

How to view a molecule in 3D | Learn MolDraw

<https://www.moldraw.com/learn/how-to-view-a-molecule-in-3d/>

Click Show 3D viewer at the bottom of the atom palette. Drag to rotate the model. Use 3D Clean Up to pose the 2D drawing.

Beginner 4 min 3 steps

Short answer: Click Show 3D viewer at the bottom of the atom palette. Drag to rotate the model. Use 3D Clean Up to pose the 2D drawing.

You will learn to: Draw cyclohexane; Open the 3D viewer; Use 3D Clean Up.

1 Watch demo 2 Try in editor

Watch the demo

3D in about 15 seconds.

The steps in text

Step 1: Draw cyclohexane

1. Open the C6 ring menu and pick **Flat C6**.
2. Click an empty spot.

Step 2: Open the 3D viewer

1. Click **Show 3D viewer** at the bottom of the atom palette. It shows two arrows.

Step 3: Use 3D Clean Up

1. Click **3D Clean Up** in the tools row. It is the cube button.

Try it in the editor

Chapter complete

Next: How to export a structure for a paper or slides

[Next chapter](#)

The full MolDraw editor opens here. It loads when you open this tab.

Questions and answers

How do I rotate my molecule?

Drag inside the 3D viewer.

What does 3D Clean Up do?

It poses the 2D drawing in perspective, so you can show depth on the canvas.

Can I export the 3D model?

Yes. The 3D viewer has its own download menu.

For more detail, read [the guide in the docs](#).

How to view a protein structure from the PDB | Learn MolDraw

<https://www.moldraw.com/learn/how-to-view-a-protein-structure-from-the-pdb/>

Open the 3D viewer here, then load a protein by its PDB ID in the full editor.

Beginner 4 min 3 steps

Short answer: Open the 3D viewer here, then load a protein by its PDB ID in the full editor.

You will learn to: Open the 3D viewer; Load a PDB entry; Change the display style.

1 Watch demo 2 Try in editor

Watch the demo

The 3D viewer in about 10 seconds.

The steps in text

Step 1: Draw benzene

1. Click the benzene button in the ring bar. Click the canvas.

Step 2: Open the 3D viewer

1. Click **Show 3D viewer** at the bottom of the atom palette. It shows two arrows.

Step 3: Load a protein

1. Open the [full editor](#) in a new tab.
2. Click **3D** in the tools row. Open the **Protein** tab.
3. Type **1CRN** in the PDB ID box. Click **Go**.
4. Pick **Cartoon** or **Surface** in the Display menu.
5. Come back and click

Try it in the editor

Chapter complete

Next: How to map atoms in a reaction

[Next chapter](#)

The full MolDraw editor opens here. It loads when you open this tab.

Questions and answers

What is a PDB ID?

A four-character code for a structure in the Protein Data Bank, such as 1CRN.

Can I open my own file?

Yes. Use Open in the Protein tab.

For more detail, read [the guide in the docs](#).

MolDraw Tutorials | Video Guides for the Free Chemistry Drawing App

<https://www.moldraw.com/tutorials/>

Watch MolDraw video tutorials: a quick tour of the free chemistry structure drawing app, from drawing molecules and the 3D viewer to templates and stereocenters.

By [MolDraw](#) · Video tutorial

[Play in editor](#) [Open MolDraw](#) [Watch on YouTube](#)

About this video

A quick tour of MolDraw, the free chemistry structure drawing app that runs in your browser. See how to draw molecules from elements and bonds, switch to the 3D viewer, add structures from the template library, and work with stereocenters.

Tip: **Play in editor** opens MolDraw with this video in a small floating player, so you can follow along while you draw.

In this video

1. Drawing a structure with elements and bonds
2. Switching to the 3D viewer and changing display modes
3. Adding common structures from the template library
4. Stereocenter support