

MolDraw free tools and spectrum viewers (part 1)

The spectrum viewers and the first half of the free chemistry tools: what each one does and how to use it.

MolDraw (<https://www.moldraw.com>) · Help centre: <https://www.moldraw.com/support/> · Updated 2026-10-17

Free Chemistry Tools & Calculators Online

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

40+ free chemistry tools: molar mass, equation balancer, Lewis structures, pH, SMILES to IUPAC, PDB to PDBQT and more. Runs in your browser, no sign-up.

Lab

TLC diagram

Build TLC plate diagrams with lanes, spots, solvent front, R_f labels, and SVG/PNG export.

[Open standalone tool](#)

Free Cyclic Voltammetry Viewer Online: E_{1/2}, ΔE_p, HOMO/LUMO

<https://www.moldraw.com/tools/cv-viewer/index.html>

Free online cyclic voltammetry (CV) viewer. Open CSV, CH Instruments, BioLogic, Gamry or Autolab files, find E_{pa}, E_{pc}, E_{1/2} and ΔE_p, convert reference electrodes, estimate HOMO/LUMO and run a Randles-Sevcik scan-rate analysis.

In short: Open CSV, CH Instruments, BioLogic, Gamry or Autolab files, find E_{pa}, E_{pc}, E_{1/2} and ΔE_p, convert reference electrodes, estimate HOMO/LUMO and run a Randles-Sevcik scan-rate analysis. It is free, works in your web browser and needs no download.

Open cyclic voltammograms, pick a cycle and read E_{pa}, E_{pc}, E_{1/2}, ΔE_p and i_{pa}/i_{pc} in plain words. Convert reference electrodes, estimate HOMO and LUMO, and check diffusion with a scan-rate series. Your files stay on your device.

Open CV file(s)

or drop them here. CSV/TXT, CH Instruments, BioLogic .txt, Gamry .DTA or Autolab ASCII. Pick several files for a scan-rate series.

Load example:

Add to the plot instead of replacing · Examples are simulated and free to reuse. [Download the sample .csv](#).

US convention Drag a box to zoom, scroll or pinch to zoom. Double-click to reset. Oxidation current is plotted up (IUPAC). Tick US convention to flip.

Reference and units

Data vs Show vs Ferrocene $E^{1/2}$ vs data ref (V) Electrode area (cm²) Current density

0.0707 cm² is a 3 mm diameter disc.

Peaks

HOMO / LUMO from onset potentials Use oxidation onset Use reduction onset Mark onsets Fc/Fc⁺ level (eV below vacuum) Scan-rate analysis (Randles-Sevcik) Electrons n Concentration (mM)

How to use the cyclic voltammetry viewer

1. Open your file(s), or press an example button.
2. Pick what the data was measured against and what you want to show. Enter your ferrocene $E^{1/2}$ if you have it.
3. Choose a cycle. Read E_{pa} , E_{pc} , $E^{1/2}$, ΔE_p and i_{pa}/i_{pc} , and the note under the table.
4. For energy levels, open HOMO / LUMO. Tick the onsets you want to use.
5. For a scan-rate series, open several files, check each scan rate, then open Scan-rate analysis.
6. Export a PNG or CSV.

Reading a cyclic voltammogram

The potential sweeps up and back while the current is recorded. An **anodic peak** (E_{pa}) shows oxidation and a **cathodic peak** (E_{pc}) shows reduction. For a reversible one-electron couple, $E^{1/2} = (E_{pa} + E_{pc})/2$ is close to the formal potential, ΔE_p is about 59 mV at 25 °C and i_{pa}/i_{pc} is about 1. A larger ΔE_p means slower electron transfer. A missing return peak means the product reacts away.

Peak current grows with $\sqrt{v}$ for diffusing species (**Randles-Sevcik**) and with v for species fixed on the electrode. For organic semiconductors the onset potentials vs Fc/Fc⁺ give rough **HOMO** and **LUMO** levels.

Frequently asked questions

Is my data uploaded?

No. Files are read and drawn in your browser only.

Which files can I open?

CSV or TXT with potential and current columns (time and cycle columns are optional), CH Instruments text exports, BioLogic EC-Lab .txt exports, Gamry .DTA files and Autolab NOVA ASCII exports. Current units (A, mA, μ A, nA) are read from the column header.

How are the peaks and ipa/ipc found?

The first peak is measured from the charging baseline, extended under the peak. The return peak uses Nicholson's method, which allows for the current still decaying from the first peak. ΔE_p near 59 mV (one electron, 25 °C) and ipa/ipc near 1 point to a reversible couple.

How do I convert between reference electrodes?

Pick what your data was measured against and what you want to show. The tool uses SCE = +0.241 V, Ag/AgCl (sat. KCl) = +0.197 V and Ag/AgCl (3 M KCl) = +0.210 V vs SHE. For Fc/Fc⁺, enter the ferrocene $E^{1/2}$ you measured in your own cell. Otherwise +0.40 V vs SCE (acetonitrile) is assumed.

How are HOMO and LUMO estimated?

From the onset potentials vs Fc/Fc⁺: $E(\text{HOMO}) = -(E_{\text{ox, onset}} + 4.8) \text{ eV}$ and $E(\text{LUMO}) = -(E_{\text{red, onset}} + 4.8) \text{ eV}$. The 4.8 eV value is a common convention for the Fc/Fc⁺ level below vacuum. Some papers use 5.1 eV, so you can change it. These are estimates, not exact orbital energies.

What does the Randles-Sevcik analysis tell me?

For a species that diffuses to the electrode, the peak current grows with the square root of the scan rate. The slope of $\log i_p$ against $\log v$ is then about 0.5, and the tool gives the diffusion coefficient D . A slope near 1 means the species is fixed on the surface (adsorbed or a film).

MolDraw Tools Hub | Free Chemistry Tools

<https://www.moldraw.com/tools/free-chem-tools/>

MolDraw free chemistry tools directory with XYZ to SMILES, chemical reaction drawer, mass spectrum predictor, XYZ/Gaussian to 2D structure, name to structure, formula to structure, structure to SMILES, converters, calculators, pKa, percent yield, grams to moles, Lipinski, druglikeness, LogP, TPSA, Lewis structure generator, viewers, and lab utilities.

SMILES to Structure

[Open tool](#)

Free IR Spectrum Viewer Online: Open JCAMP-DX, CSV and SPC Files

<https://www.moldraw.com/tools/ir-viewer/index.html>

Free online IR viewer. Open JCAMP-DX, CSV or SPC infrared spectra in your browser, switch %T and absorbance, correct the baseline, pick peaks, see functional groups and compare two spectra.

In short: Open JCAMP-DX, CSV or SPC infrared spectra in your browser, switch %T and absorbance, correct the baseline, pick peaks, see functional groups and compare two spectra. It is free, works in your web browser and needs no download.

Open an infrared spectrum, switch between %T and absorbance, clean the baseline and pick peaks. Each peak gets a likely **functional group** with a short reason. Compare two spectra on one plot. Your files stay on your device.

Open IR file

or drop it here (drop two files to compare). JCAMP-DX (.jdx, .dx), CSV or TXT (cm-1, intensity), or SPC.

Load example:

Examples are simulated from typical band positions, so they are free to reuse. [Download the sample .jdx](#) (compressed JCAMP-DX).

Main: Compare with:none Open 2nd file Drag a box to zoom. Scroll or pinch to zoom. Tap a peak to see its band. Double-click to reset. Baseline correction Show group bands Threshold 10%

How to use the IR viewer

1. Open your file, or press an example button.
2. Press %T or Absorbance to change the y axis. Tick Baseline correction if the background slopes.
3. Peaks are picked for you. Move the Threshold slider for more or fewer. Choose Add peak and tap a band to add one.
4. Read the table. Each peak shows its best functional group, the usual range and why it fits. Tap a row to shade that band.
5. Open a second file or example under Compare with to overlay two spectra.
6. Export a PNG for your report, or CSV files of the data and the peak list.

How the group matching works

Each peak is looked up in the same correlation table as the [IR spectroscopy chart](#), built from standard textbook ranges. Then the whole spectrum is used as a check. A carboxylic acid needs a very broad O-H band and a C=O band. An ester needs C=O near 1740 cm⁻¹ and a strong C-O band. Nitro and sulfone groups need both of their bands. Rare groups are only shown first when their checks pass. Anything that fails a check is marked possible.

IR alone rarely proves a structure. Use it with [NMR](#) and mass spectra, and treat the fingerprint region (below 1500 cm⁻¹) with care.

Frequently asked questions

Is my spectrum uploaded anywhere?

No. The file is read and drawn inside your browser. Nothing is sent to MolDraw.

Which files can I open?

JCAMP-DX (.jdx, .dx), including compressed data, two-column CSV or TXT (wavenumber, intensity), and SPC files in the common new format. Wavelength in micrometres is changed to cm⁻¹ for you.

How does it name the functional groups?

Each picked peak is looked up in the same correlation table as the MolDraw IR chart. The whole spectrum is then used as a check. For example, a carboxylic acid needs both a very broad O-H band and a C=O band near 1700 cm⁻¹. Matches that fail a check are marked possible.

What does baseline correction do?

It fits a rubber-band line under the spectrum, in absorbance, and takes it away. This removes a sloping or curved background so peak heights compare fairly. The plot is labelled Baseline corrected.

How do I switch between transmittance and absorbance?

Press %T or Absorbance. The tool converts with $A = -\log_{10}(T)$, so you can open a %T file and view it as absorbance, or the other way round.

Can I compare two spectra?

Yes. Open a second file under Compare with, or pick an example. Both traces are drawn on the same axis in different colours. Swap makes the second one the main spectrum for peak picking.

Free Mass Spectrum Viewer Online: Isotope Pattern, Adducts, ppm

<https://www.moldraw.com/tools/mass-spec-viewer/index.html>

Free online mass spectrum viewer. Open JCAMP-DX, CSV, mzML or mzXML files, label peaks, overlay the isotope pattern of a formula, SMILES or peptide, check adducts, ppm error and neutral losses, and export PNG or CSV.

In short: Open JCAMP-DX, CSV, mzML or mzXML files, label peaks, overlay the isotope pattern of a formula, SMILES or peptide, check adducts, ppm error and neutral losses, and export PNG or CSV. It is free, works in your web browser and needs no download.

Open a mass spectrum, label the peaks, and compare it with the isotope pattern of your formula, [SMILES](#) or peptide. Check adducts, ppm error and neutral losses. Your files stay on your device.

Open mass spectrum

or drop it here. JCAMP-DX (.jdx, .dx), CSV/TXT (m/z, intensity), mzML or mzXML (first spectrum).

Load example:

Examples are simulated and free to reuse. [Download the sample .jdx](#).

Drag a box to zoom, scroll or pinch to zoom, tap a peak to use it for the ppm error. Double-click to reset. Base peak = 100% Isotope overlay Mirror (theory below) Neutral losses Labels10

Main peaks

Tap a row to use it as the measured m/z.

Neutral losses

ppm error

Measured m/z Theoretical m/z

Common adducts

Formula, SMILES or peptide

IonPattern

How to use the mass spectrum viewer

1. Open your file, or press an example button.
2. Pick Stick or Profile, zoom to the area you want and tick Base peak = 100% to normalise.
3. Type a formula, SMILES or peptide and pick the ion, such as $[M+H]^+$. The red sticks show the theoretical isotope pattern.
4. Tap the measured peak to get the ppm error. The adduct table shows which common ions are present.
5. Read the neutral loss labels between the main peaks.
6. Export a PNG or CSV.

Reading a mass spectrum

Each peak is an ion at its **m/z** (mass divided by charge). The tallest peak is the **base peak** and is set to 100%. In EI spectra the molecular ion M^+ is often small and fragments carry the story. In ESI you mostly see $[M+H]^+$, $[M+Na]^+$ or $[M-H]^-$, and big molecules such as peptides also show 2+ and 3+ ions, with isotope peaks 0.5 or 0.33 apart.

Isotopes: carbon-13 adds a peak 1 above M, about 1.1% per carbon. Chlorine and bromine add strong peaks 2 above M. **Neutral losses** such as -18 (H_2O), -28 (CO), -44 (CO_2) or -35 (Cl) between peaks show which groups break off.

Frequently asked questions

Is my data uploaded?

No. Files are read and drawn in your browser only.

Which files can I open?

JCAMP-DX mass spectra (peak tables and continuous data), CSV or TXT with m/z and intensity columns, and mzML or mzXML. For mzML and mzXML the first spectrum is shown. Compressed (zlib) arrays work in current browsers.

What is the difference between monoisotopic, average and exact mass?

Monoisotopic mass uses the most common isotope of each element (^{12}C , ^1H , ^{35}Cl). Average mass uses natural abundances and is what you weigh on a balance. Exact m/z is the monoisotopic mass of the ion you see, with the added or removed atoms and the electron mass.

How do I check for chlorine or bromine?

Enter the formula and look at the pattern. One Cl gives an M+2 peak about one third of M (3:1). One Br gives M and M+2 about equal (1:1). Two Br give 1:2:1. The red sticks show the theory over your data.

How is the ppm error worked out?

$\text{ppm} = (\text{measured} - \text{theoretical}) / \text{theoretical} \times 1\,000\,000$. Tap a peak to use it as the measured value. For high-resolution data, within about 5 ppm is a good match.

What are the neutral loss labels?

The tool looks at the gaps between the main peaks and names common small neutral losses such as H_2O , NH_3 , CO , CO_2 , CH_3 , HCl , Cl and Br . Isotope peaks are skipped. At unit resolution CO and C_2H_4 look the same, so both may be listed.

Where do the isotope numbers come from?

Isotope masses and natural abundances are public reference values from [IUPAC](#) (CIAAW) and NIST. The pattern is worked out by combining the isotopes of every atom.

Free NMR Viewer Online: Open JCAMP-DX, CSV and Bruker Spectra

<https://www.moldraw.com/tools/nmr-viewer/index.html>

Free online NMR viewer. Open JCAMP-DX (.jdx, .dx), CSV/TXT or Bruker 1r files in your browser, zoom, pick peaks, integrate, reference, find solvent impurities and export PNG.

In short: Open JCAMP-DX (.jdx, .dx), CSV/TXT or Bruker 1r files in your browser, zoom, pick peaks, integrate, reference, find solvent impurities and export PNG. It is free, works in your web browser and needs no download.

Open a ¹H or ¹³C NMR spectrum, zoom in, pick peaks, integrate and reference it. Then find solvent and grease peaks and hide them for a clean figure. Your file stays on your device.

Open spectrum file

or drop it here. JCAMP-DX (.jdx, .dx), CSV or TXT (ppm, intensity), or Bruker (zip of the folder, or the 1r and procs files together).

Load example:

Examples are simulated spectra with real solvent and impurity shifts, so Find impurities shows hits right away. [Download the sample .jdx](#).

Edited for display. Some impurity peaks are hidden with a straight baseline. Your file is not changed. Show original in grey Drag a box to zoom. Scroll to zoom, Shift+scroll for peak height. Two fingers to zoom on a phone. Double-click to reset. Spectrometer MHz Exports show what is on screen. A cleaned spectrum is labelled as edited.

Find impurities

Solvent $\pm$ ppm

Peaks

Threshold 3%

Integrals

First integral =

Reference (shift calibration)

Peak at should be

How to use the NMR viewer

1. Open your file, or press an example button to try it.
2. Drag across the plot to zoom. Choose Pan to slide left and right. Double-click to see the whole spectrum.
3. Peaks are picked for you. Move the Threshold slider for more or fewer. Choose Pick peak to add one by clicking.
4. Choose Integrate and drag across a peak. Set "First integral =" to the number of H it stands for.
5. Press Reference to solvent so the solvent peak sits at its true value.
6. Pick your solvent and press Find impurities. Tick or untick a result to show its marks. Press Remove to hide its peaks.
7. Export a PNG for your report, or CSV and JCAMP-DX for other programs.

About the impurity table

Shifts for ^1H and ^{13}C come from Fulmer, Miller, Sherden, Gottlieb, Nudelman, Stoltz, Bercaw and Goldberg, "NMR Chemical Shifts of Trace Impurities: Common Laboratory Solvents, Organics, and Gases in Deuterated Solvents Relevant to the Organometallic Chemist", *Organometallics* 2010, 29, 2176-2179 ([doi:10.1021/om100106e](https://doi.org/10.1021/om100106e)). It extends Gottlieb, Kotlyar and Nudelman, *J. Org. Chem.* 1997, 62, 7512. The table covers about 45 common solvents, reagents, greases and gases in 12 deuterated solvents.

Removing an impurity is a display edit. It draws a straight line across that compound's peaks. Do not use a cleaned spectrum as raw data in a paper or thesis. Report the impurities instead.

Frequently asked questions

Is my spectrum uploaded to a server?

No. The file is read and plotted inside your browser. Nothing is sent to MolDraw or anyone else.

Which file types can I open?

JCAMP-DX (.jdx, .dx) including compressed (ASDF) data, two-column CSV or TXT files with ppm and intensity, and Bruker processed data: a zip of the experiment folder, or the 1r and procs files picked together.

How does Find impurities work?

Pick the deuterated solvent. The tool looks at your peaks and lists common lab solvents and reagents whose known shifts sit within your tolerance, using the published tables of Fulmer et al. (*Organometallics* 2010).

What does Remove do?

It draws a straight baseline across the peaks of that impurity, only for display and export. Your file is not changed. The plot is marked Edited for display, and Undo or Restore all brings the peaks back.

Why does the MHz setting matter?

Peaks are in ppm, but coupling constants are in Hz. On a 60 MHz magnet a 7 Hz triplet is about 0.23 ppm wide. On 600 MHz it is about 0.023 ppm wide. The MHz value also sets the Hz readout.

How do I reference my spectrum?

Press Reference to solvent to put the residual solvent peak at its listed value (7.26 ppm for CDCl_3), press TMS = 0 ppm, or click Reference, click a peak and type its true ppm.

Protein Viewer with Sequence and Chain Controls

<https://www.moldraw.com/tools/protein-viewer/index.html>

Load PDB by ID or file, inspect amino-acid sequences, style individual chains, and style selected sequence regions.

In short: Load PDB by ID or file, inspect amino-acid sequences, style individual chains, and style selected sequence regions. It is free, works in your web browser and needs no download.

Load proteins by PDB ID or upload `.pdb`, inspect amino-acid sequence, style individual chains, and right-click selected sequence regions to restyle or hide them.

PDB ID Default Chain Style Ready.

Chains

Load a protein to list chains.

Amino Acid Sequence

Drag across residues to select a region. Right-click selection to restyle or hide only that segment.

Load a protein to show sequence.

Exploring a protein structure

The Protein Data Bank (PDB) holds experimentally determined 3D structures of proteins, nucleic acids, and their complexes. Each entry has a four-character ID, for example 1CRN for crambin, a small plant protein often used in examples, or 4HHB for human deoxyhaemoglobin.

Choosing a display style

- **Cartoon:** shows secondary structure, with helices as ribbons or spirals and β -strands as arrows. Best for seeing the overall fold.
- **Stick:** shows individual bonds. Best for side chains, ligands, and active sites.
- **Sphere:** space-filling atoms that show shape and packing.
- **Line:** lightweight wireframe, useful for large structures.

Working with chains and sequences

Many structures contain several chains, for example haemoglobin's two α and two β chains. Style each chain differently to see how they pack together. Selecting a stretch of the amino-acid sequence and restyling it is a quick way to highlight a binding loop or a mutation site for a figure.

Tip: export PNG for slides, or PDB/XYZ/OBJ when you need the coordinates or a mesh in another program. To turn a bound ligand into SMILES, see [PDB to SMILES](#).

Free Raman Spectrum Viewer Online: Baseline, Peaks, Bands

<https://www.moldraw.com/tools/raman-viewer/index.html>

Free online Raman viewer. Open JCAMP-DX, CSV or SPC Raman spectra, convert nm to Raman shift, remove fluorescence and cosmic-ray spikes, smooth, pick peaks with band assignments and export PNG or CSV.

In short: Open JCAMP-DX, CSV or SPC Raman spectra, convert nm to Raman shift, remove fluorescence and cosmic-ray spikes, smooth, pick peaks with band assignments and export PNG or CSV. It is free, works in your web browser and needs no download.

Open Raman spectra, turn an nm axis into Raman shift, take away the fluorescence background and cosmic-ray spikes, smooth, pick peaks and see the likely bands. Overlay several spectra. Your files stay on your device.

Open Raman file(s)

or drop them here. JCAMP-DX (.jdx, .dx), CSV/TXT (shift or nm, intensity) or SPC. Pick several files to overlay them.

Load example:

Add to the plot instead of replacing · Examples are simulated and free to reuse. [Download the sample .jdx](#).

Normalise Show before and baseline Drag a box to zoom, scroll or pinch to zoom. Double-click to reset.

Laser and x axis

Laser File x axis is wavelength in nm

Clean up

Remove spikes threshold Savitzky-Golay smooth window order Baseline Stiffness λ p Order Peak prominence 5%

Peaks and likely bands (selected spectrum)

How to use the Raman spectrum viewer

1. Open your file(s), or press an example button.
2. If the x axis is in nm, pick your laser so the tool can work out the Raman shift.
3. Tick Remove spikes to clear cosmic rays, and Savitzky-Golay smooth if the data is noisy.
4. Pick a baseline to remove fluorescence. Check the red dashed line sits under the peaks.
5. Read the peak table. For carbon samples, read the D, G and 2D check.
6. Open more files and tick Normalise to compare them.
7. Export a PNG or the cleaned CSV.

Reading a Raman spectrum

The **Raman shift** is the energy lost by the laser light, in cm^{-1} . It is the same for any laser, so spectra from 532 and 785 nm lasers line up. Bands that change polarisability are strong: $\text{C}=\text{C}$, $\text{C}\equiv\text{C}$, $\text{S}-\text{S}$, aromatic ring breathing near 1000 cm^{-1} and symmetric stretches. Polar groups such as $\text{C}=\text{O}$ and $\text{O}-\text{H}$ are weak.

Carbon: the G band near 1580 cm^{-1} comes from sp^2 carbon, the D band near 1350 cm^{-1} needs defects or edges, and the 2D band near 2700 cm^{-1} shows the number of layers.

Silicon gives one sharp band at 520.7 cm^{-1} , which is often used to check the calibration.

Frequently asked questions

Is my data uploaded?

No. Files are read and drawn in your browser only.

Which files can I open?

JCAMP-DX (.jdx, .dx), CSV or TXT with two columns, and Thermo/Galactic SPC (new format). The x axis can be Raman shift in cm^{-1} or the absolute wavelength in nm.

My file is in nm. How do I get the Raman shift?

Pick your laser (532, 633, 785 or 1064 nm, or type your own). The tool uses $\text{shift} = 10^7/\lambda_{\text{laser}} - 10^7/\lambda$. If the tool did not notice the nm axis, tick File x axis is wavelength in nm.

How do I remove the fluorescence background?

Choose a baseline. Asymmetric least squares (ALS) follows curved backgrounds well: a bigger λ gives a stiffer line. Polynomial fits a smooth curve under the peaks; order 3 to 5 suits most spectra. The red dashed line shows what will be taken away.

What does spike removal do?

Cosmic rays make sharp spikes one or two points wide. The tool finds points that jump far above their neighbours and fills them in from the sides. Real Raman bands are wider, so they are kept. Raise the threshold if a real narrow band is touched.

How are bands assigned?

Each peak is checked against a table of common Raman ranges, such as ring breathing near 1000 cm^{-1} , $\text{C}=\text{C}$ near 1600, $\text{C}\equiv\text{C}$ near 2200, $\text{S}-\text{S}$ near 510, Si at 520 and the carbon D, G and 2D bands. If C-H stretch peaks are present the tool uses organic groups, otherwise carbon and inorganic bands. Treat the result as a guide.

Can it tell graphene from graphite?

It gives the D/G and 2D/G height ratios and the 2D width. A strong, narrow 2D band (2D/G above about 1.5, width below about 45 cm^{-1}) points to single-layer graphene. A weak or broad 2D band points to multilayer graphene or graphite.

Free TGA and DSC Viewer Online: DTG, Onset, Tg, ΔH , Crystallinity

<https://www.moldraw.com/tools/tga-dsc-viewer/index.html>

Free online TGA and DSC viewer. Open CSV, TA Instruments, NETZSCH or METTLER text exports, find TGA steps with onset, DTG peak and mass loss, and read DSC Tg, melting and crystallisation peaks with ΔH and % crystallinity.

In short: Open CSV, TA Instruments, NETZSCH or METTLER text exports, find TGA steps with onset, DTG peak and mass loss, and read DSC Tg, melting and crystallisation peaks with ΔH and % crystallinity. It is free, works in your web browser and needs no download.

Open thermogravimetric (TGA) and differential scanning calorimetry (DSC) data. Find TGA steps with onset, DTG peak and mass loss, and read Tg, melting and crystallisation with ΔH and % crystallinity. Your files stay on your device.

Open TGA / DSC file(s)

or drop them here. CSV/TXT, TA Instruments, NETZSCH or METTLER text exports.

Load example:

Add to compare instead of replacing · Examples are simulated and free to reuse. [Download the sample TA text file.](#)

Segment X axis Drag a box to zoom, scroll or pinch to zoom, double-click to reset.

Settings

PlotIn the file, endothermic is Heating rate (K/min)Sample mass (mg) DTG smoothing (°C)DSC baseline

DSC crystallinity

Polymer $\Delta H_{100\%}$ (J/g)Polymer fraction w (%)

Presets are typical literature values for $\Delta H_{100\%}$. Published numbers spread, so check the one your field uses.

How to use the TGA and DSC viewer

1. Open one or more files, or press an example button.
2. Pick TGA, DSC or TGA + DSC, and the heating or cooling segment.
3. Check the heating rate, the sample mass and which way endothermic is in your file.
4. Read the TGA steps: onset, midpoint, DTG peak, mass loss and residue.
5. Read the DSC events: Tg, melting and crystallisation with onset, peak and ΔH . Zoom to a peak and press Integrate current view to add one by hand.
6. For crystallinity, pick a polymer or type $\Delta H_{100\%}$, and set the polymer fraction for filled samples.
7. Tick Add to compare to overlay more runs, then export a PNG or CSV.

Reading TGA and DSC curves

TGA (thermogravimetric analysis) weighs a sample while it heats. Each drop is a mass-loss step, such as water, solvent or decomposition. The **DTG** curve, the derivative of mass with temperature, turns each step into a peak, which makes overlapping steps easy to see. The mass left at the end is the residue, for example ash, filler or an oxide.

DSC (differential scanning calorimetry) measures the heat flow into a sample. The **glass transition (T_g)** is a step in the curve. **Melting** is an endothermic peak and **crystallisation** an exothermic one. The peak area gives the enthalpy ΔH in J/g, and comparing it with $\Delta H_{100\%}$ gives the **crystallinity** of a polymer. A pure metal such as indium checks the temperature and enthalpy calibration.

Frequently asked questions

Is my data uploaded?

No. Files are read and analysed in your browser only.

Which files can I open?

CSV or TXT with temperature (or time), mass or mass % and heat flow columns, TA Instruments Universal Analysis or TRIOS text exports (Sig lines and StartOfData), NETZSCH Proteus ASCII exports (## header line) and METTLER STARe table exports (Index, t, T_s, Value). Mass in mg is turned into % of the starting mass.

How is the TGA onset found?

With the tangent method. The tool draws the tangent at the steepest point of the step (the DTG peak) and finds where it meets the flat plateau before the step. The endset uses the plateau after the step. The midpoint is where half of the step's mass has gone.

Which way is endothermic?

Files differ. TA Instruments usually stores endotherms as negative (exo up). NETZSCH and METTLER usually store them as positive. The tool guesses from the file type and from the biggest peak. You can change "In the file, endothermic is" and pick endo up or exo up for the plot.

How is ΔH calculated?

The peak area above the baseline, divided by the heating rate. With heat flow in W/g and the rate in K/min, ΔH (J/g) = area (W·°C/g) × 60 / rate. Choose a straight (linear) baseline, or a sigmoid baseline for peaks where the baseline level changes across the peak.

How is % crystallinity calculated?

$X_c = (\Delta H_m - |\Delta H_{cc}|) / (\Delta H_{100\%} \times w) \times 100$. ΔH_m is the melting enthalpy, ΔH_{cc} the cold crystallisation enthalpy, $\Delta H_{100\%}$ the enthalpy of a fully crystalline polymer and w the

polymer weight fraction (100% if unfilled). The $\Delta H_{100\%}$ presets are typical literature values. Published values differ, so state the one you used.

Can I compare runs or show TGA and DSC together?

Yes. Tick Add to compare and open more files to overlay several runs. The TGA + DSC view puts mass on the left axis and heat flow on the right axis, for simultaneous (SDT/STA) data or two separate runs.

Free UV-Vis Spectrum Viewer: $\lambda_{\max}$, Beer-Lambert, Colour and Tauc Band Gap

<https://www.moldraw.com/tools/uv-vis-viewer/index.html>

Free online UV-Vis viewer. Open JCAMP-DX or CSV spectra, find lambda max, calculate molar absorptivity or concentration, see the sample colour, overlay series and get a Tauc band gap.

In short: Open JCAMP-DX or CSV spectra, find lambda max, calculate molar absorptivity or concentration, see the sample colour, overlay series and get a Tauc band gap. It is free, works in your web browser and needs no download.

Open UV-Vis spectra, find $\lambda_{\max}$, work out molar absorptivity or concentration with Beer-Lambert, see the colour of the sample, overlay a whole series and find a band gap with a Tauc plot. Your files stay on your device.

Open UV-Vis file(s)

or drop them here. JCAMP-DX (.jdx, .dx) or CSV/TXT (wavelength, absorbance or %T). Pick several files to overlay them.

Load example:

Add to the plot instead of replacing · Examples are simulated and free to reuse. [Download the sample .jdx](#).

Drag a box to zoom, scroll or pinch to zoom, tap to set the cursor for Beer-Lambert. Double-click to reset. Normalise each spectrum Peak prominence4%

$\lambda_{\max}$ peaks (selected spectrum)

Tap a row to use that $\lambda_{\max}$ in the Beer-Lambert box.

Beer-Lambert: $A = \epsilon \cdot l \cdot c$

Path l (cm) Concentration or ϵ ($\text{L mol}^{-1} \text{cm}^{-1}$) Tauc plot and band gap Transition Fit from (eV)to

Absorbance stands in for the absorption coefficient α , which is fine for finding where the line meets zero. For films or powders, use α or the Kubelka-Munk function for the best numbers.

How to use the UV-Vis spectrum viewer

1. Open your file(s), or press an example button.
2. Switch between absorbance and %T, and between nm, eV and cm⁻¹.
3. Read the λ_{max} table. Tap a row, or tap the plot, to pick the wavelength for Beer-Lambert.
4. Enter the path length and concentration to get ϵ , or ϵ to get the concentration.
5. For a series, open several files and tick Normalise if you want to compare shapes.
6. For a semiconductor, open Tauc plot and band gap, choose direct or indirect and read E_g .
7. Export a PNG or CSV.

What the numbers mean

λ_{max} is the wavelength where a band absorbs most. Longer conjugated systems absorb at longer λ_{max} . **Beer-Lambert** says $A = \epsilon \cdot l \cdot c$, so with A, path length and concentration you get the molar absorptivity ϵ , or with ϵ you get the concentration. Keep A below about 1.5 for good numbers.

Colour: a sample that absorbs blue light (435 to 480 nm) looks yellow, because we see the light that is left. The table uses the standard colour wheel. **Tauc plot:** plot $(A \cdot h\nu)^2$ for a direct gap or $(A \cdot h\nu)^{1/2}$ for an indirect gap against photon energy, fit the straight edge and read the band gap where the line meets zero.

Frequently asked questions

Is my data uploaded?

No. Files are read and drawn in your browser only.

Which files can I open?

JCAMP-DX (.jdx, .dx) and CSV or TXT with two columns. The x column can be nm, μm , cm⁻¹ or eV and y can be absorbance or transmittance. The tool works out which from the headers or the numbers.

How do I overlay a titration or dilution series?

Pick several files at once, or tick Add to the plot and open more. Each gets its own colour. Tick Normalise to compare band shapes, and tap a name to make it the selected spectrum.

How is the molar absorptivity worked out?

From $A = \epsilon \cdot l \cdot c$ at the λ_{max} or at the wavelength you tap. Enter the path length (usually 1 cm) and the concentration. Enter ϵ instead to get the concentration.

How does the Tauc band gap work?

The tool turns wavelength into photon energy, plots $(A \cdot h\nu)^2$ for a direct gap or $(A \cdot h\nu)^{1/2}$ for an indirect gap, finds the steepest straight part of the edge and extends it to zero. You can

set the fit range yourself.

Why does my sample look a different colour from the one shown?

The colour comes from the strongest visible band and the colour wheel. Real colour also depends on band width, concentration and the light source, so treat it as a guide.

Free XPS Viewer and Peak Fitting Online: Shirley, Doublets, Atomic %

<https://www.moldraw.com/tools/xps-viewer/index.html>

Free online XPS viewer. Open CSV, VAMAS (.vms) or CasaXPS text, charge correct to C 1s, subtract a Shirley or linear background, fit Gaussian-Lorentzian peaks with spin-orbit doublets, get atomic % and identify elements in a survey.

In short: Open CSV, VAMAS (.vms) or CasaXPS text, charge correct to C 1s, subtract a Shirley or linear background, fit Gaussian-Lorentzian peaks with spin-orbit doublets, get atomic % and identify elements in a survey. It is free, works in your web browser and needs no download.

Open XPS spectra, charge correct to C 1s, subtract a Shirley background and fit peaks with spin-orbit doublets. Get atomic % from the areas and find elements in a survey scan. Your files stay on your device.

Open XPS file

or drop it here. VAMAS (.vms), CasaXPS text export or CSV/TXT.

Load example:

Examples are simulated and free to reuse. [Download the sample .vms](#) (survey, C 1s and O 1s).

Energy axis Source Charge shift (eV) toeV Binding energy runs from high to low, as is usual for XPS. Drag a box to zoom, scroll or pinch to zoom, double-click to reset.

Region and background

Core levelBackground

Peak fit

Same FWHM for all peaks Fit %L too

Lock (🔒) keeps a value fixed while fitting. In Move peak mode, drag a peak on the plot to set its position and height. Doublet partners keep their split and area ratio.

Elements in the survey

Atomic % from fitted regions

How to use the XPS viewer

1. Open a VAMAS, CasaXPS or CSV file, or press an example button.
2. If your file uses kinetic energy, set the energy axis to Kinetic and pick Al or Mg K α .
3. Press Set from C 1s to charge correct, or type the shift.
4. Pick a region. Set the core level (for example C 1s), the background and the fit window.
5. Press Auto peaks, or use Add peak and tap the plot. For C 1s you can load the template. Then press Fit.
6. Edit, lock or drag peaks, set doublets, and press Fit again. Check the residual line under the spectrum.
7. Read the atomic % box, or the element list for a survey, and export a PNG or CSV with the fit table.

Reading an XPS spectrum

XPS (X-ray photoelectron [spectroscopy](#)) measures the energy of electrons knocked out of the top few nanometres of a sample. Each element has core levels at known **binding energies**, so a survey scan tells you which elements are there. Small shifts of a peak, the **chemical shift**, tell you the chemical state: C-C, C-O, C=O and O-C=O in a polymer, or Si and SiO₂ on a wafer.

To compare states, remove the background (usually **Shirley**) and fit the peak with components. p, d and f levels split into **spin-orbit doublets** with a fixed split and area ratio, for example Fe 2p_{3/2} and Fe 2p_{1/2}. Dividing each area by a **sensitivity factor** gives the atomic %. These numbers depend on your instrument, so use them as estimates unless you have your own factors.

Frequently asked questions

Is my data uploaded?

No. Files are read, fitted and drawn in your browser only.

Which files can I open?

VAMAS .vms files (the ISO 14976 standard most XPS software can export, regular scans), CasaXPS text exports with K.E. or B.E. columns, and plain CSV or TXT with an energy column and an intensity column. Files with several regions show each region as a tab.

How do I convert kinetic energy to binding energy?

Set the energy axis to Kinetic and pick the X-ray source. The tool uses $BE = h\nu - KE$ with $h\nu = 1486.6$ eV for Al K α or 1253.6 eV for Mg K α , or a value you type. The spectrometer work function is assumed to be included in the calibration, as most instruments do.

How does charge correction work?

Insulating samples charge up, so every peak moves by the same amount. The usual fix is to move the C-C / C-H peak of adventitious carbon to 284.8 eV. Press Set from C 1s, or type the

shift. The reference value can be changed (some labs use 285.0 eV). This reference is a convention with known limits, so say which one you used.

What is a Shirley background?

A step-shaped background that rises on the high binding energy side of a peak, in proportion to the peak area at lower binding energy. It models electrons that lose a little energy on the way out. A linear background is a straight line between the two ends of the fit window.

What line shape is used for the peaks?

A Gaussian-Lorentzian product, GL(m), the same kind used by CasaXPS. m is the Lorentzian percentage: 0 is pure Gaussian and 100 is pure Lorentzian. 30 is a common start for polymers and oxides. Metals often need an asymmetric shape, which this tool does not model, so fit metal peaks with care.

How are spin-orbit doublets handled?

Set a peak to a p, d or f doublet and the partner peak is added at a fixed split with a fixed area ratio: 1:2 for p ($2p_{1/2} : 2p_{3/2}$), 2:3 for d and 3:4 for f. The split comes from a built-in table for common elements and can be edited.

How accurate are the atomic % values?

They are only as good as the sensitivity factors. The built-in factors are approximate Scofield-type values for Al K α and do not include your analyser transmission or escape depth. For real numbers, enter the factors from your instrument library. The survey gives a rougher estimate than fitted narrow scans.

Where do the suggested assignments come from?

3D Molecular Model Viewer - Ball and Stick & Space-Filling Models

<https://www.moldraw.com/tools/free-chem-tools/3d-molecular-model-viewer.html>

Free 3D molecule viewer: search any molecule by name, SMILES or PubChem CID and rotate a ball-and-stick, space-filling, stick or wireframe molecular model with CPK colours. Works on phones.

In short: 3D molecule viewer: search any molecule by name, SMILES or PubChem CID and rotate a ball-and-stick, space-filling, stick or wireframe molecular model with CPK colours. It is free, works in your web browser and needs no download.

Look up any molecule by name, SMILES or PubChem CID and explore it as an interactive 3D model, like a virtual molecular model kit. You can switch between ball-and-stick, space-filling, stick and wireframe, turn labels and hydrogens on or off, and save a PNG.

Quick answer: type a molecule name such as **caffeine** and drag to rotate. Ball-and-stick shows bonds and angles, space-filling shows the true size and shape, and atoms use CPK

colours (C grey, H white, O red, N blue). Molecule name, SMILES or PubChem CID Hydrogens Atom labels Spin Dark

Drag to rotate, pinch or scroll to zoom, two-finger drag to move.

SMILES:

Molecular model styles explained

Model	What it shows	Best for
Ball-and-stick	Atoms as small spheres, bonds as sticks	Bond angles, geometry and connectivity (classroom molecular model kits)
Space-filling (CPK)	Atoms at their van der Waals radii	Real size and shape, steric bulk, how molecules pack
Stick	Bonds only, coloured by atom	Larger molecules, conformations
Wireframe	Thin lines for bonds	Big structures, fast rotation

CPK colours

Atoms are coloured with the standard CPK (Jmol) scheme: carbon grey, hydrogen white, oxygen red, nitrogen blue, sulfur yellow, phosphorus orange, chlorine green, bromine dark red and iodine purple.

For your own SMILES with export to SDF, PDB or XYZ, use the [SMILES to 3D structure converter](#) . For proteins and PDB entries, use the [protein viewer](#) .

Drawing structures for your notes? MolDraw is a free online chemical structure editor for molecules, reactions and lab diagrams.

[Open MolDraw editor](#)

Frequently asked questions

What is a ball-and-stick model?

A ball-and-stick model shows atoms as coloured spheres and bonds as sticks. It makes bond angles and molecular geometry easy to see, for example the 104.5° bend of water or the tetrahedral shape of methane.

What is the difference between ball-and-stick and space-filling models?

Ball-and-stick shrinks the atoms to show the bonds and angles. A space-filling (CPK) model draws each atom at its van der Waals radius, so it shows the real size and shape of the molecule but hides the bonds.

What do the colours in a molecular model mean?

Most models use CPK colours: carbon is grey or black, hydrogen white, oxygen red, nitrogen blue, sulfur yellow, chlorine green and phosphorus orange.

How do I view a molecule in 3D?

Type its name (e.g. caffeine), a SMILES string or a PubChem CID and press Show 3D model. Drag to rotate, pinch to zoom, and switch between ball-and-stick, space-filling, stick and wireframe.

Where do the 3D structures come from?

From PubChem's computed 3D conformers. Some salts, metal complexes and very large molecules have no 3D conformer, so a 2D layout is shown instead.

Can I build my own molecule?

Yes. Use the Build a Molecule tool to put atoms together kit-style, or draw any structure in the MolDraw editor and view it in 3D.

Related chemistry tools

Ball-and-stick theme 2D ball-and-stick **MEP plugin** Electrostatic potential **SMILES Notation Guide** Related tool **IR Spectroscopy Chart (Correlation Table)** Related tool **3D models of common molecules** Water, glucose, caffeine & more **Build a molecule** Molecule builder with challenges **VSEPR molecular geometry calculator** Shapes and bond angles **SMILES to 3D structure** Export SDF, PDB, XYZ **Protein viewer** PDB entries in 3D **Name to structure** Name → 2D structure **Lewis structure generator** Dot structures **Interactive periodic table** Elements and data

AP Chemistry Score Calculator (2026) - Estimate Your 1-5

<https://www.moldraw.com/tools/free-chem-tools/ap-chemistry-score-calculator.html>

Free AP Chem score calculator: enter multiple-choice correct (out of 60) and FRQ points (out of 46) to estimate your composite and 1-5 AP Chemistry score, with cutoffs and official distributions.

In short: AP Chem score calculator: enter multiple-choice correct (out of 60) and FRQ points (out of 46) to estimate your composite and 1-5 AP Chemistry score, with cutoffs and official distributions. It is free, works in your web browser and needs no download.

Enter your multiple-choice and free-response results from a practice exam to estimate your AP Chemistry score from 1 to 5. The calculator uses the current exam format (60 MCQ + 7 FRQ, each worth 50%) and tells you how many more points you need for the next score.

Quick answer: $\text{composite} = \text{MCQ} \times 50/60 + \text{FRQ} \times 50/46$. On the estimated scale, about **72/100 earns a 5**, 58 a 4 and 42 a 3. For example, 50 MCQ correct with 30 FRQ points gives about 74, an estimated **5**. Section I: multiple-choice correct (out of 60) Q1 (long, 0-10) Q2 (long, 0-10) Q3 (long, 0-10) Q4 (short, 0-4) Q5 (short, 0-4) Q6 (short, 0-4) Q7 (short, 0-4) Section II: total FRQ points (out of 46)

Cutoffs are **estimates**. College Board does not publish fixed raw-score cutoffs. Scores are set each year so a 5 means the same thing from year to year.

AP Chemistry exam format and scoring

Section	Questions	Time	Raw points	Weight
I: Multiple choice	60	90 min	60 (no penalty for wrong answers)	50%
II: Free response	7: 3 long (10 pts) + 4 short (4 pts)	105 min	46	50%

Composite (0–100) = MCQ correct $\times$ 50/60 + FRQ points $\times$ 50/46

Estimated composite score cutoffs

Composite (out of 100)	Estimated AP score
72–100	5 (extremely well qualified)
58–71	4 (well qualified)
42–57	3 (qualified)
27–41	2 (possibly qualified)
0–26	1 (no recommendation)

Source: these ranges follow the conversion published with College Board's AP Chemistry practice exam (current 60 MCQ + 7 FRQ format). Real cutoffs move a few points from year to year, so a result within about 3 points of a boundary could go either way.

Official score distributions

Year	5	4	3	2	1	3 or higher	Mean
2025	17.8%	28.6%	31.5%	15.9%	6.2%	77.9%	3.36
2024	17.9%	27.4%	30.3%	16.9%	7.5%	75.6%	3.31
2023	16.0%	27.1%	32.0%	16.9%	8.0%	75.1%	3.26

Source: [College Board, AP Chemistry score distributions](#). AP® is a registered trademark of College Board, which is not affiliated with and does not endorse MolDraw.

How to raise your AP Chemistry score

- **The FRQ is worth more per point.** One FRQ point adds 1.09 composite points, while one MCQ adds 0.83. Show your work, carry units and justify each claim to pick up partial credit.
- **Master the calculation units:** stoichiometry, gas laws, equilibrium (K, K_{sp}, pH) and kinetics (half-life, rate laws) come up every year.
- **Practise structure questions:** Lewis structures, VSEPR shapes and hybridization are quick MCQ marks. Check yourself with our [Lewis structure generator](#) and [VSEPR calculator](#).
- **Never leave an MCQ blank.** There is no penalty for a wrong answer.

Drawing structures for your notes? MolDraw is a free online chemical structure editor for molecules, reactions and lab diagrams.

[Open MolDraw editor](#)

Frequently asked questions

How is the AP Chemistry exam scored?

Section I has 60 multiple-choice questions and Section II has 7 free-response questions worth 46 points. Each section is 50% of the composite score, and College Board converts the composite to a 1–5 AP score.

What composite score do you need for a 5 in AP Chemistry?

On the published practice-exam conversion, about 72 out of 100 composite points earns a 5. That is roughly 50 MCQ correct with 30 FRQ points. Real cutoffs vary slightly each year.

What is a passing score on AP Chemistry?

A 3 is generally considered passing. On the estimated scale that needs a composite of about 42 out of 100, for example 30 MCQ correct and 18 FRQ points.

How many free-response questions are on AP Chemistry?

Seven: three long questions worth 10 points each and four short questions worth 4 points each, for 46 points in total. You have 105 minutes, and a calculator is allowed.

Is this AP Chemistry score calculator accurate?

It uses the official section weights and the College Board practice-exam conversion. College Board sets the real cutoffs each year, so treat the result as an estimate, especially within a few points of a boundary.

What percentage of students get a 5 on AP Chemistry?

In 2025, 17.8% of students scored a 5 and 77.9% scored 3 or higher, with a mean score of 3.36 (College Board).

Related chemistry tools

Ideal Gas Law Calculator ($PV = nRT$) Related tool **Half-life calculator** Radioactive decay and kinetics **VSEPR molecular geometry calculator** Shapes, bond angles, hybridization **Chemical equation balancer** Balance reactions step by step **Limiting reagent calculator** Find the limiting reactant **pH calculator** pH, pOH and concentrations **Lewis structure generator** Dot structures and formal charges **Electron configuration calculator** Orbitals and noble-gas notation

Build a Molecule Online - Molecule Builder with 3D &

Challenges

<https://www.moldraw.com/tools/free-chem-tools/build-a-molecule.html>

Free online molecule builder: snap atoms together like a model kit with valence checks, get the formula, name, SMILES and 3D model live, and try 20 build-a-molecule challenges. Works on phones.

In short: Molecule builder: snap atoms together like a model kit with valence checks, get the formula, name, SMILES and 3D model live, and try 20 build-a-molecule challenges. It is free, works in your web browser and needs no download.

A virtual molecular model kit. Tap to add atoms, join them with single, double or triple bonds, and watch the formula update as you build. Valence rules stop impossible structures. Finished molecules are named, given a SMILES string and can be shown in 3D. Try challenge mode to test yourself.

Quick answer: carbon makes 4 bonds, nitrogen 3, oxygen 2 and hydrogen 1. Build **water** as H-O-H, **methane** as C with four H, and **CO₂** as O=C=O. When every orange badge is gone, the molecule is complete.

Formula	
Bonds	
Name	—
SMILES	

[Open in 3D viewer](#)

Challenge mode

Pick a molecule to build

How to build a molecule

1. **Pick an atom** from the kit (C, H, O, N, halogens, S, P, B) and tap the board to place it.
2. **With an atom selected** (dashed ring), tap the board or tap the same atom again to add a bonded atom. Choose single, double or triple first.
3. **Join two atoms** by selecting one and tapping the other. Tap a bond to change single → double → triple.
4. **Orange badges** show how many bonds an atom still needs. Use *+H fill* to complete them with hydrogens.
5. When every atom is satisfied, you get the **formula, name and SMILES**, and can view the molecule in 3D.

Valence rules used (neutral atoms)

Atom	H, F, Cl, Br, I	O	N	B	C	S	P
Bonds	1	2	3	3	4	2, 4 or 6	3 or 5

A double bond counts as 2 and a triple bond as 3. Charged species such as NH_4^+ are not part of the neutral kit.

Challenges: 20 molecules to build

Start with water, methane and ammonia, move on to double and triple bonds (CO_2 , N_2 , ethyne), then isomers. **Ethanol and dimethyl ether** are both $\text{C}_2\text{H}_6\text{O}$, and the checker tells you when you have built the right formula with the wrong connectivity. It finishes with rings (cyclopropane).

Once you have built a molecule, explore its shape with the [VSEPR calculator](#) or rotate it in the [3D molecular model viewer](#).

Drawing structures for your notes? MolDraw is a free online chemical structure editor for molecules, reactions and lab diagrams.

[Open MolDraw editor](#)

Frequently asked questions

How do I build a molecule online?

Choose an atom from the kit, tap to place it, then add bonded atoms or join atoms together. The builder checks each atom's valence, shows the formula as you go, and looks up the name when the molecule is complete.

Is this like the PhET Build a Molecule simulation?

It has the same idea, putting atoms together like a molecular model kit. It runs in any browser on phones and tablets, and adds double and triple bonds, a SMILES output, a name lookup and a 3D view.

Why can't I add another bond to an atom?

Each neutral atom has a fixed number of bonds: H 1, O 2, N 3, C 4. Once an atom's valence is full, the builder blocks extra bonds so you can only build real molecules.

What do the orange numbers mean?

They show how many more bonds an atom needs to complete its valence. Fill them with other atoms, add double bonds, or press +H fill to add hydrogens.

How does challenge mode work?

Pick a target molecule. When every atom has a full set of bonds, the builder compares your structure with the target. It even spots isomers that have the right formula but different connectivity.

Can I see my molecule in 3D?

Yes. Once it is complete and known to PubChem, press Show in 3D for a ball-and-stick model, or open it in the full 3D molecular model viewer.

Related chemistry tools

Smart Draw plugin Sketch by hand **Degree of Unsaturation Calculator** Related tool **3D molecular model viewer** Ball-and-stick & space-filling **VSEPR molecular geometry calculator** Shapes and bond angles **Lewis structure generator** Dot structures **Structure to IUPAC name** Draw → name **Formula to structure** Find structures for a formula **Interactive periodic table** Valence and groups

CAS Number to SMILES Converter

<https://www.moldraw.com/tools/free-chem-tools/cas-number-to-smiles-converter.html>

CAS Number to SMILES converter by MolDraw. Enter a CAS Registry Number such as 50-00-0 or 64-17-5 and resolve PubChem SMILES, IUPAC name, formula, molecular weight, and CID.

In short: Enter a CAS Registry Number such as 50-00-0 or 64-17-5 and resolve PubChem SMILES, IUPAC name, formula, molecular weight, and CID. It is free, works in your web browser and needs no download.

Enter a CAS Registry Number and resolve the matching compound record to SMILES, IUPAC name, formula, molecular weight, and PubChem CID.

Quick answer: Type a CAS number such as **50-00-0**, **64-17-5**, or **7732-18-5**. The tool searches PubChem synonyms and returns the best matching SMILES record. CAS Registry Number

Examples

SMILES output appears here.

Input and output formats

Input: CAS Registry Number	Output: SMILES	
Full name	CAS Registry Number	SMILES (Simplified Molecular Input Line Entry System)
What it holds	A number given to a substance by Chemical Abstracts Service. It holds no structure itself, so it is looked up.	Atoms, bonds, rings, charges and stereo as one line of text. No coordinates.
File or form	Text like 50-78-2	.smi or plain text

CAS Number Lookup Notes

CAS numbers are registry identifiers, not structure strings. This converter resolves a CAS number through public PubChem synonym records, then reads the associated SMILES and chemical metadata.

- Use the hyphenated CAS format, for example **64-17-5**.

- If a CAS number has multiple salts, mixtures, or supplier variants, verify the returned compound.
- For drawing, use the related CAS to Structure tool.

[CAS to Structure](#) [SMILES to Structure](#) [CID to SMILES](#)

Related chemistry tools

[InChI to SMILES Converter](#)[InChIKey to SMILES Converter](#)[SMILES Notation Guide](#)[Structure to SMILES Converter](#)[IUPAC Name to SMILES Converter](#)

CAS Number to Structure | Chemical Structure Lookup

<https://www.moldraw.com/tools/free-chem-tools/cas-number-to-structure.html>

CAS Number to Structure tool by MolDraw. Enter a CAS Registry Number and view the chemical structure, SMILES, formula, molecular weight, and PubChem CID.

In short: Enter a CAS Registry Number and view the chemical structure, SMILES, formula, molecular weight, and PubChem CID. It is free, works in your web browser and needs no download.

Look up a CAS Registry Number and view the matching 2D chemical structure, SMILES, formula, molecular weight, and PubChem CID.

Quick answer: Enter a CAS number such as **64-17-5** or **7732-18-5**. The page resolves a PubChem record and displays the chemical structure image. CAS Registry Number [Open in MolDraw](#)

Examples

Structure metadata appears here. Structure image appears here.

How CAS to Structure Lookup Works

CAS numbers are resolved through public PubChem synonym records. The tool then uses the matching PubChem CID to display a 2D structure image and metadata.

- Verify the result for salts, mixtures, hydrates, and ambiguous registry records.
- Use the SMILES value to open the compound in MolDraw or convert it to other identifiers.

[CAS to SMILES](#) [SMILES to Structure](#) [Molecular Weight Calculator](#)

Related chemistry tools

[Molecular Formula to Structure](#) [SearchName to Structure Tool](#)[SMILES Notation Guide](#)[Structure to SMILES Converter](#)[IUPAC Name to SMILES Converter](#)

Chemical Equation Balancer - Balance Online Free

<https://www.moldraw.com/tools/free-chem-tools/chemical-equation-balancer.html>

Balance any chemical equation instantly, including redox and ionic equations ($\text{MnO}_4^- + \text{Fe}^{2+}$). Free online chemical equation balancer with atom check.

In short: Balance any chemical equation instantly, including redox and ionic equations ($\text{MnO}_4^- + \text{Fe}^{2+}$). It is free, works in your web browser and needs no download.

Type an unbalanced equation and get the smallest whole-number coefficients, with an atom-by-atom and charge check. Handles combustion, double displacement, redox and net ionic equations with charges.

Quick answer: enter reactants and products separated by = or $\rightarrow$, for example $\text{C}_3\text{H}_8 + \text{O}_2 = \text{CO}_2 + \text{H}_2\text{O}$. The balancer returns **$\text{C}_3\text{H}_8 + 5 \text{O}_2 \rightarrow 3 \text{CO}_2 + 4 \text{H}_2\text{O}$** . Unbalanced equation
The balanced equation appears here.

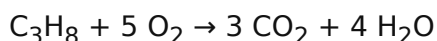
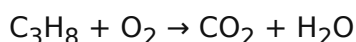
Separate species with + (put spaces around + when you use ions). Write charges at the end: Fe^{3+} , SO_4^{2-} or SO_4^{2-} , MnO_4^- . Coefficients you type are ignored and recalculated.

How to use the chemical equation balancer

1. Type the reactants, an arrow (=, $\rightarrow$ or $\rightarrow$), then the products, for example $\text{Fe} + \text{O}_2 = \text{Fe}_2\text{O}_3$.
2. Check every formula is correct, because the balancer cannot fix a wrong product. Use capital letters for element symbols.
3. Click *Balance equation*. You get the smallest whole-number coefficients and a table showing equal atoms (and charge) on both sides.
4. Copy the result, or send it to the [limiting reagent calculator](#) or the [net ionic equation calculator](#).

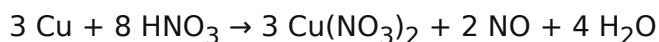
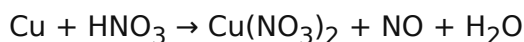
Worked examples

Propane combustion

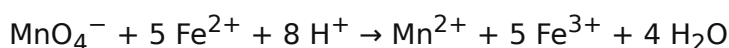
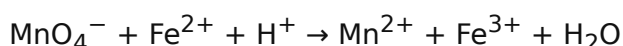


C: 3 = 3, H: 8 = 8, O: 10 = 6 + 4.

Copper with nitric acid (redox)



Permanganate oxidising iron(II)



Charge: +17 on both sides.

How the balancer works

Balancing means choosing coefficients so that every element, and the total charge, is the same on both sides (conservation of mass and charge). The tool writes one equation per element. For $a + b \rightarrow c + d$, carbon gives $a \cdot C_a = c \cdot C_c$, and so on. It then solves the system exactly with fractions, the algebraic method, and scales the answer to the smallest whole numbers. This is the same result you get by inspection or by the half-reaction method, but it never misses a solution.

Σ (coefficient $\times$ atoms of element) on the left = Σ on the right, for every element and for charge

Balancing by hand (inspection method)

1. Balance elements that appear in only one reactant and one product first (C, then H in combustion).
2. Leave free elements such as O_2 , H_2 or Fe until last.
3. If you end with a fraction (e.g. $7/2 O_2$), multiply every coefficient by 2.
4. Check atoms and charge once more.

When an equation cannot be balanced

If an element appears on only one side, or the only solution needs a negative coefficient, the reaction as written is impossible: a formula is wrong or a product is missing. Some equations are combinations of two independent reactions (for example $H_2 + O_2 \rightarrow H_2O + H_2O_2$). These have infinitely many balances, and the tool warns you and shows the smallest one.

Need a clean reaction scheme for a report? Draw structures, arrows and conditions in the free MolDraw reaction drawer.

[Draw the reaction](#)

Frequently asked questions

How do you balance a chemical equation?

Write the correct formulas, then change only the coefficients (never subscripts) until each element and the total charge are equal on both sides. This tool does it automatically with exact algebra.

Can this balance redox reactions?

Yes. Enter the full molecular equation ($KMnO_4 + HCl = KCl + MnCl_2 + H_2O + Cl_2$) or the ionic form with charges ($MnO_4^- + Fe^{2+} + H^+ = Mn^{2+} + Fe^{3+} + H_2O$); electrons are balanced through the charge equation.

How do I type charges and states?

Put the charge at the end of the formula: Na⁺, Fe³⁺, SO₄²⁻ (or SO₄2-), MnO₄⁻. State symbols such as (aq), (s), (g) and (l) are accepted and ignored for balancing.

Why does it say the equation cannot be balanced?

Usually a formula is wrong, a product is missing, or an element appears on only one side. Check the formulas and that reactants and products are on the correct sides.

Can coefficients be fractions?

Balanced equations are normally written with the smallest whole numbers. Fractions such as 7/2 O₂ are sometimes used in thermochemistry, but this tool reports whole numbers.

What about the net ionic equation?

Use the net ionic equation calculator. It balances the equation, splits strong electrolytes into ions and cancels spectator ions.

Related chemistry tools

Stoichiometry calculator Grams, moles and gas volumes
Theoretical yield calculator Limiting reagent → grams of product
AP Chemistry score calculator Estimate your 1–5 exam score
Net ionic equation calculator Complete and net ionic equations
Limiting reagent calculator Limiting reactant and theoretical yield
Oxidation number calculator Oxidation states with steps

Draw a Chemical Reaction Free | Reaction Drawer

<https://www.moldraw.com/tools/free-chem-tools/chemical-reaction-drawer.html>

Draw a chemical reaction free in your browser. Sketch reactants, an arrow, products, and conditions, then export. Open an aldol, Wittig, or Suzuki example and edit it.

Aldol condensation

Two acetaldehydes to the aldol product.

[Draw aldol reaction](#)

CID to SMILES Converter

<https://www.moldraw.com/tools/free-chem-tools/cid-to-smiles-converter.html>

PubChem CID to SMILES converter by MolDraw. Resolve compound IDs to canonical SMILES strings for chemistry workflows.

In short: Resolve compound IDs to canonical SMILES strings for chemistry workflows. It is free, works in your web browser and needs no download.

Convert PubChem CID values to canonical SMILES identifiers.

SMILES output appears here.

Input and output formats

Input: PubChem CID	Output: SMILES	
Full name	PubChem CID	SMILES (Simplified Molecular Input Line Entry System)
What it holds	The Compound ID of a record in the PubChem database. It is looked up to get the structure.	Atoms, bonds, rings, charges and stereo as one line of text. No coordinates.
File or form	A whole number like 2244	.smi or plain text

File Format Explained

PubChem CID is a numeric compound identifier used by PubChem. It points to a database record rather than directly encoding molecular structure.

SMILES is a compact line notation for molecular connectivity. Converting CID to SMILES is useful when a database gives a PubChem ID but your drawing or cheminformatics tool expects a structure string.

CID lookup depends on PubChem records. Different compound records, salts, isotopes, or stereochemical forms may have different CIDs and SMILES strings.

About PubChem CIDs

A PubChem Compound ID (CID) is the numeric identifier PubChem assigns to each unique chemical structure in its database. For example, aspirin is CID 2244 and caffeine is CID 2519. Papers, supplier catalogues, and datasets often cite CIDs, but a number on its own does not tell you the structure. Converting it to SMILES gives you an editable structure string.

How to use it

1. Enter one CID (digits only, no "CID" prefix).
2. Run the conversion to fetch the canonical SMILES from PubChem.
3. Copy the SMILES into MolDraw, a spreadsheet, or another converter.

FAQ

Is a CID the same as a CAS number? No. CAS Registry Numbers are assigned by the Chemical Abstracts Service and have a hyphenated format such as 50-78-2; CIDs are PubChem's own sequential numbers. **Why does a salt give a dotted SMILES?** Salts and mixtures contain separate components, which SMILES writes with a dot, for example [Na+].[Cl-].

Next steps: draw it with [SMILES to Structure](#) or get an identifier with [SMILES to InChIKey](#).

Related chemistry tools

[CAS Number to SMILES Converter](#)[InChI to SMILES Converter](#)[InChIKey to SMILES Converter](#)[IUPAC Name to SMILES Converter](#)[SMILES Notation Guide](#)[Structure to SMILES Converter](#)

Degree of Unsaturation Calculator (IHD / DBE) - Rings + π Bonds

<https://www.moldraw.com/tools/free-chem-tools/degree-of-unsaturation-calculator.html>

Free degree of unsaturation calculator: get the IHD/DBE from any molecular formula (N, O, halogens, ions) or SMILES/name, with rings vs π -bond breakdown and step-by-step working.

In short: Degree of unsaturation calculator: get the IHD/DBE from any molecular formula (N, O, halogens, ions) or SMILES/name, with rings vs π -bond breakdown and step-by-step working. It is free, works in your web browser and needs no download.

Find the degree of unsaturation, also called the index of hydrogen deficiency (IHD) or double bond equivalents, from a molecular formula. Nitrogen, oxygen, sulfur, halogens and ions are handled. Enter a SMILES string or compound name to see exactly how many rings and π bonds the molecule has.

Quick answer: $\text{DoU} = \text{C} - (\text{H} + \text{X})/2 + \text{N}/2 + 1$. Benzene C_6H_6 gives **4** (1 ring + 3 π bonds), pyridine $\text{C}_5\text{H}_5\text{N}$ gives 4, and $\text{C}_4\text{H}_9\text{Br}$ gives 0. Molecular formula

Formulas may include N, O, S, P, B, Si, halogens and a charge (NH_4^+ , $\text{C}_2\text{H}_3\text{O}_2^-$). A SMILES or name also gives the split into rings and π bonds. Drawing a structure? Use [structure to SMILES](#) first.

Degree of unsaturation formula

The degree of unsaturation (DoU), also called the **index of hydrogen deficiency (IHD)**, double bond equivalents (DBE) or rings plus double bonds (RDB), counts how many pairs of hydrogen atoms a molecule is "missing" compared with a saturated, open-chain compound. Each ring and each π bond removes two hydrogens.

$$\text{DoU} = \text{C} - (\text{H} + \text{X})/2 + \text{N}/2 + 1$$

- **C:** carbon (and other tetravalent atoms such as Si).
- **H and X:** hydrogens and halogens (F, Cl, Br, I). A halogen takes one bond, just like H.
- **N:** nitrogen (and other trivalent atoms such as P and B). Each one adds a half.
- **O and S are ignored:** a divalent atom slots into a chain without changing the hydrogen count. CH_3CH_3 and CH_3OCH_3 both have DoU 0.

Equivalent form: $\text{DoU} = (2\text{C} + 2 + \text{N} - \text{H} - \text{X}) / 2$.

What each unit means

Feature	Adds to DoU	Example
Ring	1	Cyclohexane $C_6H_{12} = 1$
C=C or C=O double bond	1	Ethene $C_2H_4 = 1$, acetone $C_3H_6O = 1$
Triple bond ($C\equiv C$, $C\equiv N$)	2	Ethyne $C_2H_2 = 2$
Benzene ring	4 (1 ring + 3 π)	Benzene $C_6H_6 = 4$
Naphthalene	7 (2 rings + 5 π)	$C_{10}H_8 = 7$

Worked examples

1. **C_4H_9Br** : $4 - (9 + 1)/2 + 0 + 1 = 0$. Saturated, acyclic: a bromobutane.
2. **C_5H_5N (pyridine)**: $5 - 5/2 + 1/2 + 1 = 4$. One ring plus three π bonds, aromatic like benzene.
3. **$C_9H_8O_4$ (aspirin)**: $9 - 8/2 + 1 = 6$. Benzene ring (4) + two C=O (2). Oxygens are ignored.
4. **C_8H_8** : DoU = 5. It could be styrene (benzene ring + one C=C) or cubane (5 rings). The DoU narrows the possibilities, and IR/NMR decide between them.

Ions and odd results

For an ion, add half the charge: $DoU = C - (H + X)/2 + N/2 + 1 + q/2$. This works for N-, O- and S-centred ions such as pyridinium $C_5H_6N^+$ (4), ammonium NH_4^+ (0) and acetate $C_2H_3O_2^-$ (1). A carbocation, though, comes out one higher than its rings plus π bonds, because the empty p orbital counts as a unit. A **half-integer** answer for a neutral formula means a radical or a typo. A **negative** answer means no structure exists.

Using DoU in structure determination

Work out the DoU first, then use spectroscopy. A DoU of 4 or more usually signals an aromatic ring (check the IR for C=C stretches near 1600 and 1500 cm^{-1} and the ^1H NMR for signals at 6.5–8 ppm). A DoU of 1 with a strong IR band near 1715 cm^{-1} points to a C=O rather than a ring. Get the molecular formula from an [empirical formula](#) or [exact mass](#) calculation, then list real candidates with [formula to structure](#).

Drawing structures for your notes? MolDraw is a free online chemical structure editor for molecules, reactions and lab diagrams.

[Open MolDraw editor](#)

Frequently asked questions

How do you calculate degree of unsaturation?

Use $DoU = C - (H + X)/2 + N/2 + 1$, where X is the number of halogens. Oxygen and sulfur are ignored. For C_6H_6 : $6 - 3 + 1 = 4$.

What does a degree of unsaturation of 1 mean?

The molecule has either one ring or one double bond ($C=C$, $C=O$ or $C=N$). Spectroscopy tells you which.

Why are halogens counted like hydrogen?

A halogen forms one bond, so in a formula it simply takes the place of a hydrogen atom.

Why is oxygen ignored in the DoU formula?

Oxygen forms two bonds, so inserting it into a chain ($C-O-C$ or $C-O-H$) does not change the number of hydrogens needed.

Why does nitrogen add one half?

Nitrogen forms three bonds, so each N brings one extra hydrogen position compared with a divalent atom: $+1$ H, which is $+\frac{1}{2}$ in the DoU.

Is degree of unsaturation the same as IHD or DBE?

Yes. Index of hydrogen deficiency, double bond equivalents and rings-plus-double-bonds are all names for the same number.

How do I find the number of rings and π bonds separately?

The formula alone cannot separate them. Enter a SMILES or a compound name and the calculator counts rings (bonds – atoms + 1) and gives π bonds as DoU – rings.

Related chemistry tools

[How to read an NMR spectrum](#)[Worked unknowns](#)[How to read an IR spectrum](#)[Functional groups](#)[Molecular formula finder](#)[From exact mass or CHN %](#)[IR spectroscopy chart](#)[IR correlation table](#)

Dilution Calculator ($C_1V_1 = C_2V_2$) - Free

<https://www.moldraw.com/tools/free-chem-tools/dilution-calculator.html>

Free dilution calculator using $C_1V_1 = C_2V_2$: find stock volume, final concentration or final volume. Example: 1 M to 0.1 M in 100 mL needs 10 mL stock.

In short: Dilution calculator using $C_1V_1 = C_2V_2$: find stock volume, final concentration or final volume. It is free, works in your web browser and needs no download.

1 M stock diluted to 0.1 M in 100 mL needs 10 mL of stock and 90 mL of solvent. Change the numbers to match your dilution.

Stock concentration C_1 (M) Target concentration C_2 (M) Final volume V_2 (mL) Stock volume V_1 : 10.0000 mL | Solvent to add: 90.0000 mL

How the $C_1V_1 = C_2V_2$ formula works

When you dilute a stock solution, the amount of solute stays the same, so $C_1 \times V_1 = C_2 \times V_2$. Solving for the stock volume gives $V_1 = C_2 \times V_2 \div C_1$, and the solvent to add is $V_2 - V_1$.

C_1 and C_2 must use the same unit (for example both in M or both in mM), and the result V_1 comes out in the same unit as V_2 . The target concentration must be lower than the stock concentration.

Need a figure for your report? [Draw chemical structures online](#) with MolDraw, a free [online ChemDraw alternative](#).

Related chemistry tools

[Half-Life Calculator](#)

Druglikeness Calculator | Lipinski and Veber Checks

<https://www.moldraw.com/tools/free-chem-tools/druglikeness-calculator.html>

Free druglikeness calculator for SMILES or compound names. Check Lipinski and Veber-style properties including MW, LogP, HBD, HBA, TPSA, and rotatable bonds.

In short: Druglikeness calculator for SMILES or compound names. It is free, works in your web browser and needs no download.

Enter a SMILES string or compound name to calculate a simple druglikeness guideline score from Lipinski and Veber-style properties.

Enter a compound to calculate. SMILES Compound name Results appear here.

How the Druglikeness Score Works

This tool combines six common medicinal chemistry property checks: Lipinski molecular weight, LogP, H-bond donors, H-bond acceptors, plus Veber-style TPSA and rotatable bond checks. The score is the percentage of these checks that pass.

- Use it for quick triage, teaching, and early compound comparison.
- Do not treat the score as a prediction of potency, safety, or approval likelihood.
- Natural products, macrocycles, prodrugs, and specialized target classes may fall outside these simple guidelines.

[Lipinski rule calculator](#) [LogP calculator](#) [TPSA calculator](#)

Reading the result

Druglikeness rules are quick filters that flag molecules less likely to be orally absorbed. Lipinski's rule of five, published by Lipinski and colleagues in 1997, suggests poor absorption is more likely when a compound has more than 5 H-bond donors, more than 10 H-bond

acceptors, a molecular weight over 500, or a calculated logP over 5. Veber's criteria add rotatable bonds (10 or fewer) and polar surface area (140 Å² or less).

What the rules do not tell you

- They are guidelines, not predictions of activity, toxicity, or metabolism.
- Many approved drugs break one or more rules, notably natural products, antibiotics, and drugs absorbed by transporters.
- They apply to oral delivery; injectables and topical products follow different constraints.

Example: ibuprofen (C₁₃H₁₈O₂, about 206 g/mol, one donor and two acceptors) passes the Lipinski checks comfortably. Use the score to prioritise or compare a series of analogues, then look at individual properties with the [LogP](#) and [TPSA](#) calculators.

Related chemistry tools

[ChEMBL bioactivity plugin](#)[pKa Calculator](#)[SMILES to Molecular Weight Calculator](#)[Mass Spectrum Predictor](#)

Electron Configuration Calculator - Any Element

<https://www.moldraw.com/tools/free-chem-tools/electron-configuration-calculator.html>

Get the electron configuration of any element or ion, in full and noble-gas notation, including exceptions like Cr and Cu. Shows orbital diagram. Free.

In short: Get the electron configuration of any element or ion, in full and noble-gas notation, including exceptions like Cr and Cu. It is free, works in your web browser and needs no download.

Pick an element and optional ion charge to get the ground-state electron configuration in full and noble-gas (shorthand) notation, an orbital box diagram, electrons per shell and the number of unpaired electrons. Known exceptions such as Cr, Cu, Pd and Au are built in.

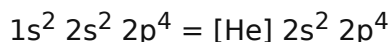
Quick answer: iron (Fe, Z = 26) is **1s² 2s² 2p⁶ 3s² 3p⁶ 3d⁶ 4s² = [Ar] 3d⁶ 4s²**. Fe³⁺ loses the 4s electrons first: [Ar] 3d⁵. Element (symbol, name or atomic number) Ion charge
Results appear here.

How to use the electron configuration calculator

1. Type an element symbol (Cu), name (copper) or atomic number (29).
2. For an ion, enter its charge: 2 for Cu²⁺, -1 for Cl⁻.
3. Read the noble-gas shorthand and the full configuration. Orbitals are listed in shell order (3d before 4s).
4. Use the orbital diagram to count unpaired electrons and predict whether the atom or ion is paramagnetic.

Worked examples

Oxygen (Z = 8)

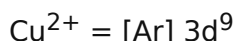


Two unpaired 2p electrons (Hund's rule).

Copper (Z = 29), an exception

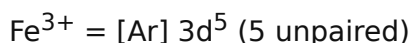
Aufbau predicts $[\text{Ar}] 3d^9 4s^2$

Actual: $[\text{Ar}] 3d^{10} 4s^1$



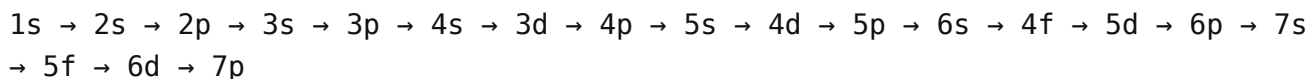
Iron(III) ion, Fe^{3+}

$\text{Fe} = [\text{Ar}] 3d^6 4s^2$; remove $2 \times 4s$ then $1 \times 3d$



How electron configurations are built

Electrons fill orbitals in order of increasing energy (the **Aufbau principle**), following the Madelung ($n + l$) rule:



Each orbital holds two electrons of opposite spin (**Pauli exclusion**), and electrons spread out singly across orbitals of the same subshell before pairing (**Hund's rule**). Capacities are $s = 2$, $p = 6$, $d = 10$ and $f = 14$.

Exceptions: Cr, Cu and others

About 20 elements have measured ground states that differ from the simple order, usually because a half-filled or completely filled d or f subshell is lower in energy. The common ones are Cr ($[\text{Ar}] 3d^5 4s^1$), Cu ($[\text{Ar}] 3d^{10} 4s^1$), Mo, Ag, Pd ($[\text{Kr}] 4d^{10}$), Pt, Au, La, Ce, Gd and several actinides. The calculator uses the experimental (NIST) ground states for these.

Ions

Anions add electrons to the next available orbital ($\text{Cl}^- = [\text{Ar}]$). Transition-metal cations lose their outer s electrons before d electrons, so Fe^{2+} is $[\text{Ar}] 3d^6$, not $[\text{Ar}] 3d^4 4s^2$.

Explore trends across the table with the [interactive periodic table](#).

Building teaching material? Draw molecules, orbitals and apparatus for your slides with the free MolDraw editor.

Frequently asked questions

What is an electron configuration?

It lists how an atom's electrons are distributed among orbitals, for example $1s^2 2s^2 2p^4$ for oxygen. Superscripts give the number of electrons in each subshell.

What is noble gas notation?

A shorthand that replaces the core electrons with the preceding noble gas in brackets: sodium $1s^2 2s^2 2p^6 3s^1$ becomes $[\text{Ne}] 3s^1$.

Why is copper $3d^{10} 4s^1$ and not $3d^9 4s^2$?

A completely filled 3d subshell is especially stable, so one 4s electron moves into 3d. Chromium does the same to reach a half-filled 3d5.

Which electrons are removed first when forming a cation?

Electrons in the highest principal shell are removed first. For transition metals the 4s electrons go before the 3d electrons.

How do you find the number of valence electrons?

For main-group elements, count the electrons in the outermost shell (highest n). For example, $[\text{Ne}] 3s^2 3p^5$ for chlorine gives 7 valence electrons.

What is the electron configuration of Fe^{3+} ?

$[\text{Ar}] 3d^5$. Iron is $[\text{Ar}] 3d^6 4s^2$, and the three electrons removed are the two 4s electrons and one 3d electron.

Related chemistry tools

AP Chemistry score calculator Estimate your 1–5 exam score
VSEPR molecular geometry calculator Shape, bond angles, hybridization in 3D
Interactive periodic table All 118 elements with data
Oxidation number calculator Oxidation states with steps
Lewis structure generator Lewis dot structures and VSEPR shape
Molar mass calculator Step-by-step molar mass working
Molecular weight calculator Formula to g/mol with % composition
Chemical equation balancer Balance reactions and redox ions
Net ionic equation calculator Complete and net ionic equations
pH calculator pH, pOH, weak acids and buffers

Need to sketch molecules for a report? [Draw chemical structures online](#) with MolDraw, a free online ChemDraw alternative (see the [ChemDraw vs MolDraw comparison](#)).

Empirical Formula Calculator - % to Formula

<https://www.moldraw.com/tools/free-chem-tools/empirical-formula-calculator.html>

Empirical and molecular formula calculator: enter percent composition or grams, get the simplest whole-number ratio and molecular formula. With steps.

In short: Empirical and molecular formula calculator: enter percent composition or grams, get the simplest whole-number ratio and molecular formula. It is free, works in your web browser and needs no download.

Enter the percent composition (or grams) of each element. The calculator converts to moles, divides by the smallest value, finds the whole-number ratio and, if you give a molar mass, the molecular formula. Every step is shown.

Quick answer: 40.0% C, 6.70% H and 53.3% O gives the mole ratio 1 : 2 : 1, so the empirical formula is **CH₂O**. With M = 180 g/mol the molecular formula is **C₆H₁₂O₆**. Molar mass of compound, g/mol (optional, for the molecular formula)

Enter mass percentages or grams from an analysis. They do not need to add up to 100.

Results appear here.

How to use the empirical formula calculator

1. Enter each element and its mass percent (or the grams found by analysis). Assume a 100 g sample, so 40.0% C means 40.0 g C.
2. The calculator divides each mass by the element's atomic mass to get moles.
3. It divides every mole value by the smallest one, then multiplies by 2, 3... if needed to reach whole numbers (e.g. 1.5 → ×2).
4. Optionally enter the compound's molar mass. $n = \text{molar mass} \div \text{empirical formula mass}$ gives the molecular formula.

Worked examples

40.0% C, 6.70% H, 53.3% O

C 3.330 mol, H 6.647 mol, O 3.332 mol
÷ 3.330 → 1 : 1.996 : 1.000

Empirical CH₂O (30.026 g/mol)

M = 180 → n = 6 → C₆H₁₂O₆

64.8% C, 13.6% H, 21.6% O

C 5.395, H 13.49, O 1.350 mol
÷ 1.350 → 3.996 : 9.993 : 1

C₄H₁₀O

(e.g. butanol or diethyl ether, 74.12 g/mol)

69.94% Fe, 30.06% O

Fe 1.2524, O 1.8789 mol $\rightarrow$ 1 : 1.500

$\times 2 \rightarrow 2 : 3$

Fe₂O₃

Empirical vs molecular formula

The **empirical formula** is the simplest whole-number ratio of atoms in a compound. The **molecular formula** is the actual number of atoms in one molecule, always a whole-number multiple of it. Glucose (C₆H₁₂O₆), formaldehyde (CH₂O) and acetic acid (C₂H₄O₂) all share the empirical formula CH₂O.

moles = mass $\div$ atomic mass $\rightarrow$ ratio = moles $\div$ smallest moles $\rightarrow$ n = M(compound) $\div$ M(empirical)

Handling ratios that are not whole numbers

Ratio ends in about...	Multiply all by
.5	2
.33 or .67	3
.25 or .75	4
.2, .4, .6, .8	5

Small deviations (± 0.1) come from rounding in experimental data and are rounded away. Large deviations usually mean a wrong percentage or a missing element: if the percentages add to less than 100, the remainder is often oxygen.

Going the other direction, formula to percent composition, is done by the [molecular weight calculator](#).

Found the molecular formula? Draw the possible isomers in MolDraw to check which structure fits your spectra.

[Draw isomers in MolDraw](#)

Frequently asked questions

How do you calculate an empirical formula from percent composition?

Treat the percentages as grams in a 100 g sample, convert each to moles, divide by the smallest number of moles and round (or multiply up) to whole numbers.

How can I calculate the molecular formula from the empirical formula?

Divide the compound's molar mass by the empirical formula mass to get n, then multiply every subscript by n. CH₂O (30.03) with M = 180 gives n = 6, C₆H₁₂O₆.

What is the empirical formula of a compound with 40.0% C, 6.70% H and 53.3% O?

CH₂O. The mole ratio is 3.33 : 6.65 : 3.33, which simplifies to 1 : 2 : 1.

What is the empirical formula of a compound that is 64.8% C, 13.6% H and 21.6% O?

C₄H₁₀O. Moles: C 5.40, H 13.5, O 1.35. Dividing by 1.35 gives 4 : 10 : 1.

What if the percentages do not add up to 100?

The calculator works with any amounts, because only the ratio matters. If an element is missing from the analysis (often oxygen), add it as 100 minus the sum.

Can the empirical and molecular formula be the same?

Yes, when $n = 1$. Water (H₂O) and carbon dioxide (CO₂) are examples.

Related chemistry tools

Molecular formula finder From exact mass or CHN %
Degree of unsaturation calculator HD / rings + π bonds
Molecular weight calculator Formula to g/mol with % composition
Molar mass calculator Step-by-step molar mass working
Grams to moles calculator Convert mass and moles
Percent yield calculator Actual vs theoretical yield
Limiting reagent calculator Limiting reactant and theoretical yield
Exact mass calculator Monoisotopic mass for MS
Chemical equation balancer Balance reactions and redox ions
Interactive periodic table All 118 elements with data

Need to sketch molecules for a report? [Draw chemical structures online](#) with MolDraw, a free online ChemDraw alternative (see the [ChemDraw vs MolDraw comparison](#)).

Exact Mass Calculator | Monoisotopic Formula Mass

<https://www.moldraw.com/tools/free-chem-tools/exact-mass-calculator.html>

Exact mass calculator by MolDraw. Enter a chemical formula and calculate monoisotopic exact mass, nominal mass, average molecular weight, and isotope breakdown.

In short: Enter a chemical formula and calculate monoisotopic exact mass, nominal mass, average molecular weight, and isotope breakdown. It is free, works in your web browser and needs no download.

Enter a chemical formula and calculate monoisotopic exact mass for mass spectrometry and formula checks.

Quick answer: exact mass uses the most abundant isotope of each element, such as C-12 and H-1, instead of average atomic weight. Chemical formula Enter a formula to calculate exact mass.

Exact Mass vs Molecular Weight

Exact mass is monoisotopic and is most useful for mass spectrometry. Molecular weight uses standard average atomic weights and is usually better for molarity, percent composition, and solution calculations.

[Protein Molecular Weight Calculator](#)[Molar Mass Calculator](#) [Molecular weight calculator](#) [SMILES to molecular formula](#) [SMILES to molecular weight](#)

Worked example

For caffeine, $\text{C}_8\text{H}_{10}\text{N}_4\text{O}_2$, the monoisotopic mass uses $^{12}\text{C} = 12.000000$, $^1\text{H} = 1.007825$, $^{14}\text{N} = 14.003074$, and $^{16}\text{O} = 15.994915$:

$8 \times 12.000000 + 10 \times 1.007825 + 4 \times 14.003074 + 2 \times 15.994915 \approx \mathbf{194.0804}$. Its average molecular weight is about 194.19 g/mol, so the two values differ in the first decimal place.

Using it with mass spectra

- In positive electrospray you usually see $[\text{M}+\text{H}]^+$: add the mass of a proton, about 1.00728, giving 195.0877 for caffeine.
- Sodium adducts $[\text{M}+\text{Na}]^+$ add about 22.98922.
- High-resolution instruments report masses to 4 or more decimals, and agreement within a few ppm supports a proposed formula.

Tip: enter formulas with correct capitalisation (Cl, not CL), because CL would be read as carbon plus an invalid symbol. To get a formula from a structure first, use [SMILES to Molecular Formula](#).

Related chemistry tools

[How to read a mass spectrum](#)[Mass Spectrum Viewer](#)[Half-Life Calculator](#)[Degree of Unsaturation Calculator](#)[IR Spectroscopy Chart \(Correlation Table\)](#)[Molecular Formula Finder](#)

Formula and Mass Tools | Molecular Weight, Formula, Exact Mass

<https://www.moldraw.com/tools/free-chem-tools/formula-and-mass-tools.html>

Formula and mass chemistry tools by MolDraw: molecular weight calculator, formula to structure search, SMILES to molecular formula, SMILES to molecular weight, exact mass, mass spectrum predictor, and grams to moles calculator.

Molecular Weight Calculator

Enter a formula such as H_2O , $\text{Ca}(\text{OH})_2$, or $\text{C}_6\text{H}_{12}\text{O}_6$ and calculate average molar mass, element breakdown, and percent composition.

Grams to Moles Calculator | Moles to Grams

<https://www.moldraw.com/tools/free-chem-tools/grams-to-moles-calculator.html>

Grams to moles and moles to grams calculator by MolDraw. Enter a formula and convert mass to moles or moles to mass using molar mass.

In short: Enter a formula and convert mass to moles or moles to mass using molar mass. It is free, works in your web browser and needs no download.

Convert grams to moles or moles to grams using the molar mass calculated from a chemical formula.

Quick answer: moles = grams / molar mass, and grams = moles × molar mass. Chemical formula Mass (grams) Result appears here.

Grams and Moles Formula

- **grams to moles:** moles = mass in grams / molar mass.
- **moles to grams:** grams = moles × molar mass.
- Molar mass is calculated from the formula using standard atomic weights.

[Molar Mass Calculator](#)[Empirical Formula Calculator](#) [Molecular weight calculator](#) [Limiting reagent calculator](#) [Percent yield calculator](#)

Worked examples

Grams to moles: how many moles are in 10.0 g of calcium carbonate, CaCO_3 ? Molar mass = $40.08 + 12.01 + 3 \times 16.00 = 100.09 \text{ g/mol}$, so $n = 10.0 \div 100.09 = \mathbf{0.0999 \text{ mol}}$.

Moles to grams: you need 0.250 mol of glucose, $\text{C}_6\text{H}_{12}\text{O}_6$ (180.16 g/mol). Mass = $0.250 \times 180.16 = \mathbf{45.0 \text{ g}}$.

Why moles matter

Balanced equations count particles, not grams. To find how much of each reagent to use, or which is the limiting reagent, convert masses to moles, compare them using the coefficients in the equation, then convert back to grams if needed.

Common mistakes

- Forgetting water of crystallisation: $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$ (249.69 g/mol) is much heavier than anhydrous CuSO_4 (159.61 g/mol).
- Using the formula of a diatomic element incorrectly: oxygen gas is O_2 (32.00 g/mol), not O.
- Rounding the molar mass too early in multi-step calculations.

For solutions, continue with the [Molarity Calculator](#).

Related chemistry tools

[Ideal Gas Law Calculator \(PV = nRT\)](#)[Theoretical Yield Calculator](#)[Stoichiometry Calculator](#)

Half-Life Calculator - Radioactive Decay & First-Order Kinetics

<https://www.moldraw.com/tools/free-chem-tools/half-life-calculator.html>

Free half-life calculator: solve for remaining amount, initial amount, time or half-life, get the decay constant k, and see a decay chart. Includes zero-, first- and second-order half-life.

In short: Half-life calculator: solve for remaining amount, initial amount, time or half-life, get the decay constant k, and see a decay chart. It is free, works in your web browser and needs no download.

Calculate radioactive decay or first-order reaction kinetics. Enter any three of the initial amount, remaining amount, time and half-life to find the fourth. You also get the decay constant, the number of half-lives, step-by-step working and a decay curve.

Quick answer: $N = N_0 \times (1/2)^{t/t_{1/2}}$. After 24.06 days, 100 g of I-131 ($t_{1/2} = 8.02$ d) has gone through 3 half-lives, so **12.5 g** remain. The decay constant is $k = 0.693 / t_{1/2}$.

Fill in any three values and leave the one you want to find **blank**.

Initial amount N_0 Remaining N Elapsed time t Half-life $t_{1/2}$ Time unit Amount unit

Half-life from a rate constant (any reaction order)

Reaction order Rate constant k $[A]_0$ (M)

Half-life formulas

$N = N_0 \times (1/2)^{(t / t_{1/2})}$ $N = N_0 \times e^{(-kt)}$ $k = \ln 2 / t_{1/2} \approx 0.693 / t_{1/2}$ $t = t_{1/2} \times \ln(N_0/N) / \ln 2$ $t_{1/2} = t \times \ln 2 / \ln(N_0/N)$ mean lifetime $\tau = 1/k = t_{1/2} / \ln 2$

Radioactive decay and every **first-order reaction** follow the same law. The half-life is constant and does not depend on how much you start with. For other reaction orders the half-life changes as the reaction proceeds:

Order	Integrated rate law	Half-life	Units of k
Zero	$[A] = [A]_0 - kt$	$t_{1/2} = [A]_0 / 2k$	$M s^{-1}$
First	$\ln[A] = \ln[A]_0 - kt$	$t_{1/2} = \ln 2 / k$	s^{-1}
Second	$1/[A] = 1/[A]_0 + kt$	$t_{1/2} = 1 / (k[A]_0)$	$M^{-1} s^{-1}$

Remaining after n half-lives

Half-lives	1	2	3	4	5	6	7	10
% remaining	50	25	12.5	6.25	3.125	1.5625	0.78125	0.0977

Common radioisotope half-lives

Isotope	Half-life	Used for
Carbon-14	5,730 years	Radiocarbon dating
Iodine-131	8.02 days	Thyroid treatment
Technetium-99m	6.01 hours	Medical imaging
Fluorine-18	109.7 minutes	PET scans
Cobalt-60	5.27 years	Radiotherapy, sterilisation
Strontium-90	28.8 years	Fission product
Caesium-137	30.1 years	Fission product
Radium-226	1,600 years	Historical radiotherapy
Uranium-238	4.47 billion years	Dating rocks
Potassium-40	1.25 billion years	K-Ar dating

Values from IAEA/NNDC nuclear data, rounded.

Worked examples

How much I-131 is left?

100 g, $t_{1/2} = 8.02$ d, after 24.06 d: $24.06/8.02 = 3$ half-lives, so $100 \times (1/2)^3$

12.5 g remain

Radiocarbon age

A sample has 25% of its original C-14. $\ln(100/25)/\ln 2 = 2$ half-lives $\times 5,730$ y

Age $\approx 11,460$ years

Find the half-life

80 mg falls to 10 mg in 30 min. $\ln(8)/\ln 2 = 3$ half-lives in 30 min

$t_{1/2} = 10$ min

First-order rate constant

$k = 1.5 \times 10^{-3} \text{ s}^{-1}$; $t_{1/2} = 0.693 / 1.5 \times 10^{-3}$

$t_{1/2} = 462 \text{ s}$ (7.7 min)

Drawing structures for your notes? MolDraw is a free online chemical structure editor for molecules, reactions and lab diagrams.

[Open MolDraw editor](#)

Frequently asked questions

How do you calculate half-life?

Use $t_{1/2} = t \times \ln 2 / \ln(N_0/N)$, where N_0 is the starting amount and N is the amount left after time t . If you know the first-order rate constant, $t_{1/2} = \ln 2 / k \approx 0.693 / k$.

How do you calculate how much remains after a given time?

$N = N_0 \times (1/2)^{(t/t_{1/2})}$. Divide the time by the half-life to get the number of half-lives, then halve the amount that many times. For example, 3 half-lives leave 12.5%.

What is the relationship between half-life and the rate constant?

For first-order processes, including radioactive decay, $k = \ln 2 / t_{1/2}$ and $t_{1/2} = 0.693 / k$. The decay constant λ is the same quantity as k .

Does half-life depend on the starting amount?

Not for first-order reactions or radioactive decay. For zero-order reactions $t_{1/2} = [A]_0/2k$, and for second-order reactions $t_{1/2} = 1/(k[A]_0)$, so it does depend on the starting concentration.

How long until only 1% remains?

About 6.64 half-lives, because $\ln(100)/\ln 2 = 6.64$. After 10 half-lives about 0.1% remains.

Can I use this for drug or caffeine half-life?

Yes. Most drugs are eliminated by first-order kinetics, so the same formula applies. Caffeine has a half-life of roughly 5 hours in healthy adults. This tool is for education, not medical advice.

Related chemistry tools

Ideal gas law calculator $PV = nRT$ and gas laws **AP Chemistry score calculator** Estimate your 1-5 exam score **Dilution calculator** $C_1V_1 = C_2V_2$ **Molarity calculator** Moles, volume and concentration **pH calculator** pH, pOH and concentrations **Exact mass calculator** Monoisotopic masses **Interactive periodic table** Elements and isotopes

Ideal Gas Law Calculator ($PV = nRT$) + Combined, Boyle, Charles

<https://www.moldraw.com/tools/free-chem-tools/ideal-gas-law-calculator.html>

Free ideal gas law calculator: solve $PV = nRT$ for pressure, volume, moles or temperature with unit conversions, plus combined, Boyle, Charles and Gay-Lussac gas laws, step by step.

In short: Ideal gas law calculator: solve $PV = nRT$ for pressure, volume, moles or temperature with unit conversions, plus combined, Boyle, Charles and Gay-Lussac gas laws, step by step. It is free, works in your web browser and needs no download.

Solve $PV = nRT$ for pressure, volume, moles or temperature in any units (atm, kPa, mmHg, psi, L, mL, °C, °F, K). Enter grams and a formula to convert to moles automatically. Switch to the combined, Boyle, Charles or Gay-Lussac law for before-and-after problems.

Quick answer: $PV = nRT$ with $R = 0.08206 \text{ L}\cdot\text{atm mol}^{-1} \text{ K}^{-1}$. One mole of gas at 0 °C and 1 atm occupies **22.41 L**. Always convert temperature to kelvin ($^{\circ}\text{C} + 273.15$).

PV = nRT. Leave the value you want to find **blank**.

Pressure unit Volume unit Temperature unit Pressure P Volume V Amount n n unit Gas formula
Temperature T $P_1V_1/T_1 = P_2V_2/T_2$

Gas law formulas

Law	Equation	Held constant
Ideal gas law	$PV = nRT$	—
Combined gas law	$P_1V_1/T_1 = P_2V_2/T_2$	n
Boyle's law	$P_1V_1 = P_2V_2$	T, n
Charles's law	$V_1/T_1 = V_2/T_2$	P, n
Gay-Lussac's law	$P_1/T_1 = P_2/T_2$	V, n
Avogadro's law	$V_1/n_1 = V_2/n_2$	P, T

Values of the gas constant R

$8.314 \text{ J mol}^{-1} \text{ K}^{-1}$	($= 8.314 \text{ Pa}\cdot\text{m}^3 \text{ mol}^{-1} \text{ K}^{-1} = 8.314 \text{ kPa}\cdot\text{L mol}^{-1} \text{ K}^{-1}$)
$0.08206 \text{ L}\cdot\text{atm mol}^{-1} \text{ K}^{-1}$	use with atm and litres
$62.36 \text{ L}\cdot\text{torr mol}^{-1} \text{ K}^{-1}$	use with mmHg/torr and litres

Always use **kelvin**: $T(\text{K}) = T(^{\circ}\text{C}) + 273.15$. At STP (0 °C, 1 atm) one mole of an ideal gas takes up 22.414 L. At IUPAC STP (0 °C, 100 kPa) it takes up 22.711 L.

Worked examples

Pressure of CO₂

22 g CO₂ (0.500 mol) in 5.00 L at 25 °C: $P = nRT/V = 0.500 \times 0.08206 \times 298.15 / 5.00$

$P = 2.45 \text{ atm}$

Boyle's law

6.0 L of gas at 1.0 atm is compressed to 3.0 atm at constant T: $V_2 = P_1V_1/P_2$

$V_2 = 2.0 \text{ L}$

Charles's law

2.00 L at 25 °C heated to 100 °C: $V_2 = 2.00 \times 373.15/298.15$

$$V_2 = 2.50 \text{ L}$$

Combined gas law

500 mL at 101.3 kPa, 20 °C goes to 85 kPa, 5 °C: $V_2 = 500 \times (101.3/85) \times (278.15/293.15)$

$$V_2 = 565 \text{ mL}$$

Drawing structures for your notes? MolDraw is a free online chemical structure editor for molecules, reactions and lab diagrams.

[Open MolDraw editor](#)

Frequently asked questions

What is the ideal gas law?

$PV = nRT$ links pressure P , volume V , amount n (mol) and temperature T (kelvin) of an ideal gas, where $R = 8.314 \text{ J mol}^{-1} \text{ K}^{-1} = 0.08206 \text{ L}\cdot\text{atm mol}^{-1} \text{ K}^{-1}$. If you know any three, you can find the fourth.

Which value of R should I use?

Match R to your units: 0.08206 for atm and L, 8.314 for kPa and L (or Pa and m^3), 62.36 for mmHg and L. This calculator converts units for you, so you can mix them.

Why must temperature be in kelvin?

Gas laws are proportional to absolute temperature. Using °C gives wrong answers, and even division by zero at 0 °C. Add 273.15 to convert °C to K.

What is the combined gas law?

$P_1V_1/T_1 = P_2V_2/T_2$ for a fixed amount of gas. Boyle's (constant T), Charles's (constant P) and Gay-Lussac's (constant V) laws are special cases.

What is the molar volume of a gas at STP?

22.414 L/mol at 0 °C and 1 atm, or 22.711 L/mol at the IUPAC standard of 0 °C and 100 kPa. At 25 °C and 1 atm it is 24.47 L/mol.

When does the ideal gas law fail?

At high pressure or low temperature, where the volume of the molecules and the attractions between them matter. Real gases then follow equations such as van der Waals.

Related chemistry tools

Stoichiometry calculator Grams, moles and gas volumes **Theoretical yield calculator** Limiting reagent → grams of product **Molar mass calculator** g/mol from a formula **Grams to moles calculator** Mass ↔ moles **Half-life calculator** Decay and first-order kinetics **Molarity calculator** Solution concentration **Limiting reagent calculator** Find the limiting reactant **AP Chemistry score calculator** Estimate your exam score

InChI to InChIKey Converter

<https://www.moldraw.com/tools/free-chem-tools/inchi-to-inchikey-converter.html>

InChI to InChIKey converter by MolDraw. Convert full InChI identifiers into compact InChIKey format for search and indexing.

In short: Convert full InChI identifiers into compact InChIKey format for search and indexing. It is free, works in your web browser and needs no download.

Convert a full InChI string into the compact InChIKey value.

InChIKey output appears here.

Input and output formats

Input: InChI	Output: InChIKey	
Full name	InChI (IUPAC International Chemical Identifier)	InChIKey
What it holds	A layered text identifier built from the structure. The standard InChI is the same in every program.	A 27 character hash of the InChI, made for web and database search. It cannot be turned back into a structure without a lookup database.
File or form	Text starting with InChI=1S/	Text like XXXXXXXXXXXXXXXX-YYYYYYYYYY-Z

File Format Explained

InChI is a full layered chemical identifier that can describe connectivity, hydrogens, charge, stereochemistry, and isotope information.

InChIKey is a shorter hashed representation of an InChI. It is easier to search and index, but it is not meant to preserve all structural layers in a readable form.

Use InChI when you need full identifier detail. Use InChIKey when you need a compact database key or search-friendly compound identifier.

InChI versus InChIKey

An InChI is a layered text description of a structure: formula, connectivity, hydrogens, charge, and stereochemistry each sit in their own layer. It is precise but long, and it contains characters such as slashes that search engines handle poorly. The InChIKey is a fixed 27-character hash of the InChI, built for web search and database indexing.

Reading an InChIKey

Aspirin's InChIKey is BSYNRYMUTXBXSQ-UHFFFA0YSA-N.

- The first block of 14 letters encodes the connectivity (the molecular skeleton).

- The second block of 10 characters encodes stereochemistry, isotopes, and other layers, plus flags for the standard InChI and version.
- The final letter encodes protonation; N means neutral.

FAQ

Can I convert an InChIKey back to a structure? Not mathematically, because a hash cannot be reversed. You need a database lookup, which is what the [InChIKey to InChI](#) tool does. **Can two molecules share an InChIKey?** Collisions are possible in theory but extremely rare in practice. Stereoisomers share the first block but differ in the second.

Related chemistry tools

[InChI to SMILES Converter](#) [MOL to InChIKey Converter](#) [SDF to InChIKey Converter](#) [SMILES Notation Guide](#) [SMILES to Structure Converter Online](#) [Structure to SMILES Converter](#)

InChI to SMILES Converter

<https://www.moldraw.com/tools/free-chem-tools/inchi-to-smiles-converter.html>

InChI to SMILES converter by MolDraw. Convert InChI identifiers to canonical SMILES strings.

In short: Convert InChI identifiers to canonical SMILES strings. It is free, works in your web browser and needs no download.

Convert InChI strings from literature and databases into SMILES format.

SMILES output appears here.

Input and output formats

Input: InChI	Output: SMILES	
Full name	InChI (IUPAC International Chemical Identifier)	SMILES (Simplified Molecular Input Line Entry System)
What it holds	A layered text identifier built from the structure. The standard InChI is the same in every program.	Atoms, bonds, rings, charges and stereo as one line of text. No coordinates.
File or form	Text starting with InChI=1S/	.smi or plain text

File Format Explained

InChI is the IUPAC International Chemical Identifier. It is layered, deterministic, and useful for describing molecular formula, connectivity, hydrogens, charge, stereochemistry, and isotopes.

SMILES is shorter and easier to paste into many drawing, search, and cheminformatics tools. Converting InChI to SMILES is helpful when a database gives InChI but your workflow expects SMILES.

Different services may return different canonical SMILES for the same InChI. Treat equivalent SMILES strings as valid if they describe the same molecule.

When to convert InChI to SMILES

InChI is excellent for identifying a compound unambiguously, but most drawing programs, cheminformatics scripts, and search boxes expect SMILES. Converting lets you take an identifier from a database record or a paper's supplementary data and turn it into something you can edit and draw.

How to use it

1. Paste a full InChI string, including the InChI=1S/ prefix.
2. Convert, then copy the SMILES output.
3. Paste the SMILES into MolDraw to see and edit the structure.

Example

Ethanol: InChI=1S/C2H6O/c1-2-3/h3H,2H2,1H3 becomes CC0. The InChI lists the formula, the connectivity layer (atoms 1-2-3), and where the hydrogens are; SMILES expresses the same molecule in three characters.

FAQ

Will stereochemistry be kept? If the InChI contains stereo layers (/t, /m, /s or /b), they are translated into SMILES @ or / and \ symbols. **Why is my SMILES different from another tool's?** One molecule can have several valid SMILES; compare them by converting both to an InChIKey with [SMILES to InChIKey](#).

Related chemistry tools

[SMILES to InChI Converter](#)[CAS Number to SMILES Converter](#)[CID to SMILES Converter](#)[InChI to InChIKey Converter](#)[SMILES Notation Guide](#)[SMILES to Structure Converter Online](#)

InChIKey to InChI Converter

<https://www.moldraw.com/tools/free-chem-tools/inchikey-to-inchi-converter.html>

InChIKey to InChI converter by MolDraw. Resolve an InChIKey into a full InChI string using public chemistry identifiers.

In short: Resolve an InChIKey into a full InChI string using public chemistry identifiers. It is free, works in your web browser and needs no download.

Resolve an InChIKey into a full InChI string through PubChem.

InChI output appears here.

Input and output formats

Input: InChIKey	Output: InChI	
Full name	InChIKey	InChI (IUPAC International Chemical Identifier)
What it holds	A 27 character hash of the InChI, made for web and database search. It cannot be turned back into a structure without a lookup database.	A layered text identifier built from the structure. The standard InChI is the same in every program.
File or form	Text like XXXXXXXXXXXXXXX-YYYYYYYYY-Z	Text starting with InChI=1S/

File Format Explained

InChIKey is a fixed-length hashed key made from an InChI. It is excellent for searching databases, but the full InChI cannot be mathematically recovered from the key alone.

InChI is the full International Chemical Identifier and carries readable structural layers. This converter resolves the InChIKey through PubChem when a matching record is available.

If no match is found, the compound may be absent from the lookup database or the InChIKey may refer to a different protonation, stereochemical, or isotopic form.

How this lookup works

An InChIKey is a one-way hash, so it cannot be decoded into a structure directly. This tool resolves the key against a chemical database and returns the full InChI of the matching record. If no database knows the compound, there is no way to recover the structure from the key alone.

How to use it

1. Paste a 27-character InChIKey in the format XXXXXXXXXXXXXXX-XXXXXXXXXX-X.
2. Run the lookup.
3. Use the InChI in other tools, or convert onward with [InChI to SMILES](#).

Example

Caffeine's InChIKey RYYVLZVUVIJJVGH-UHFFFA0YSA-N resolves to InChI=1S/C8H10N4O2/c1-10-4-9-6-5(10)7(13)12(3)8(14)11(6)2/h4H,1-3H3.

Troubleshooting

- Check for missing hyphens or extra spaces copied from a PDF.
- Newly made or proprietary compounds may not be in public databases.
- If you only know the first 14-character block, search it in a database to list all stereoisomers that share that skeleton.

Related chemistry tools

[InChI to InChIKey Converter](#)[InChIKey to SMILES Converter](#)[MOL to InChI Converter](#)[SDF to InChI Converter](#)[SMILES Notation Guide](#)[SMILES to Structure Converter Online](#)

InChIKey to SMILES Converter

<https://www.moldraw.com/tools/free-chem-tools/inchikey-to-smiles-converter.html>

InChIKey to SMILES converter by MolDraw. Resolve InChIKey identifiers to canonical SMILES strings.

In short: Resolve InChIKey identifiers to canonical SMILES strings. It is free, works in your web browser and needs no download.

Resolve InChIKey identifiers to canonical SMILES using PubChem PUG REST.

SMILES output appears here.

Input and output formats

Input: InChIKey	Output: SMILES	
Full name	InChIKey	SMILES (Simplified Molecular Input Line Entry System)
What it holds	A 27 character hash of the InChI, made for web and database search. It cannot be turned back into a structure without a lookup database.	Atoms, bonds, rings, charges and stereo as one line of text. No coordinates.
File or form	Text like XXXXXXXXXXXXXXXX-YYYYYYYYYY-Z	.smi or plain text

File Format Explained

InChIKey is a compact hashed chemical identifier often used for database lookup and web search. It is not an editable structural notation by itself.

SMILES is an editable one-line structure string. This converter uses the InChIKey to find a matching compound record and then returns a SMILES representation.

Because InChIKey lookup depends on database records, unusual salts, mixtures, stereoisomers, or unmatched compounds may not resolve cleanly.

Why look up SMILES from an InChIKey

InChIKeys appear in many databases, patents, and supplementary files because they are short and searchable. To draw or modify the compound, you need a structure format; SMILES is the most convenient. This tool finds the record that matches the key and returns its SMILES.

How to use it

1. Paste the full InChIKey, for example BSYNRYMUTXBXSQ-UHFFFAOYSA-N for aspirin.
2. Convert to get the SMILES, here CC(=O)OC1=CC=CC=C1C(=O)O.
3. Paste the SMILES into MolDraw or [SMILES to Structure](#) to view it.

FAQ

Why is the lookup sometimes empty? The key must exist in a public database. Keys for unpublished or proprietary compounds will not resolve. **Does the last letter matter?** Yes. It records protonation state, so a neutral acid and its deprotonated form have different keys. **What about stereoisomers?** Enantiomers share the first 14 characters but differ in the second block, so use the complete key to get the correct isomer.

Related chemistry tools

[SMILES to InChIKey Converter](#)[CAS Number to SMILES Converter](#)[CID to SMILES Converter](#)[InChI to SMILES Converter](#)[SMILES Notation Guide](#)[Structure to SMILES Converter](#)

Interactive Periodic Table - All 118 Elements

<https://www.moldraw.com/tools/free-chem-tools/interactive-periodic-table.html>

Free interactive periodic table with all 118 elements: atomic mass, electron configuration, electronegativity, density and ionization energy. Searchable.

Rows 9 and 10 display lanthanides and actinides. Data source includes all known elements (1-118).

IR Spectroscopy Chart & Table - Interactive IR Correlation Table

<https://www.moldraw.com/tools/free-chem-tools/ir-spectroscopy-chart.html>

Interactive IR spectroscopy chart: look up any peak (cm^{-1}), filter the IR correlation table by functional group, and read intensity and shape for C=O, O-H, N-H, C $\equiv$ N and more. Values from Pavia and Silverstein.

In short: Interactive IR spectroscopy chart: look up any peak (cm^{-1}), filter the IR correlation table by functional group, and read intensity and shape for C=O, O-H, N-H, C $\equiv$ N and more. It is free, works in your web browser and needs no download.

A searchable infrared absorption table for organic functional groups. Type a peak position to see which groups absorb there, or filter by class to compare carbonyls, amines, alkynes and more. Every band lists its wavenumber range, intensity, shape and the partner peaks that confirm it.

Quick answer: the key IR peaks are O-H 3400–3200 (broad), N-H 3500–3300, C-H 3000–2850 (sp^3) or 3100–3000 (sp^2), C $\equiv$ N $\approx$ 2250, C $\equiv$ C $\approx$ 2150, **C=O $\approx$ 1715** (ketone), C=C 1680–

1600 and C-O 1300-1000 cm^{-1} . Find a peak (cm^{-1}) $\pm$ tolerance Functional group class Search

· Bars run from 4000 cm^{-1} (left) to 400 cm^{-1} (right), as on a real spectrum. Darker bars are stronger bands.

IR spectroscopy correlation table

Class	Functional group / vibration	Wavenumber (cm^{-1})	Intensity / shape	Notes
Alkanes	Alkane C-H C-H stretch (sp^3)	2850-3000	Strong sharp	Almost every organic compound shows peaks just below 3000 cm^{-1} .
Alkanes	CH₂ bend C-H bend (scissoring)	1450-1470	Medium sharp	$\approx 1465 \text{ cm}^{-1}$.
Alkanes	CH₃ bend C-H bend (umbrella)	1370-1380	Medium sharp	$\approx 1375 \text{ cm}^{-1}$. A gem-dimethyl or isopropyl group splits it into a doublet.
Alkenes	Alkene =C-H =C-H stretch (sp^2)	3000-3100	Medium sharp	Just above 3000 cm^{-1} , which separates it from alkane C-H.
Alkenes	Alkene C=C C=C stretch	1600-1680	Weak-medium sharp	Weak or absent in symmetric trans or tetrasubstituted alkenes. Conjugation lowers it.
Alkenes	Alkene =C-H bend =C-H out-of-plane bend	650-1000	Strong sharp	Pattern shows substitution: monosubstituted ≈ 990 and 910 ; trans ≈ 970 ; 1,1-disubstituted ≈ 890 .
Alkynes	Terminal alkyne $\equiv\text{C-H}$ $\equiv\text{C-H}$ stretch (sp)	3260-3330	Strong sharp	Strong and narrow near 3300 cm^{-1} . Narrower than O-H or N-H.
Alkynes	Alkyne C$\equiv\text{C}$ C $\equiv\text{C}$ stretch	2100-2260	Weak-medium sharp	Weak. Absent in symmetric internal alkynes.
Aromatics	Aromatic C-H C-H stretch (sp^2)	3000-3100	Weak-medium sharp	Often several small peaks just above 3000 cm^{-1} .
Aromatics	Aromatic C=C C=C ring stretch	1585-1600	Medium sharp	Usually paired with a band near 1500-1450 cm^{-1} .
Aromatics	Aromatic C=C C=C ring stretch	1450-1500	Medium sharp	Second ring-stretch band.

Class	Functional group / vibration	Wavenumber (cm ⁻¹)	Intensity / shape	Notes
Aromatics	Aromatic overtones Overtone / combination bands	1667-2000	Weak sharp	Weak pattern of bands that reveals the ring substitution pattern.
Aromatics	Aromatic C-H bend C-H out-of-plane bend	690-900	Strong sharp	Monosubstituted: ≈ 750 and ≈ 690 ; ortho ≈ 750 ; para ≈ 830 ; meta ≈ 780 and ≈ 690 (plus ≈ 880).
Alcohols & phenols	Alcohol O-H (H-bonded) O-H stretch	3200-3400	Strong broad	Broad, rounded band in neat liquids and solids.
Alcohols & phenols	Alcohol O-H (free) O-H stretch	3600-3650	Medium sharp	Only in dilute solution or the gas phase.
Alcohols & phenols	Alcohol C-O C-O stretch	1000-1260	Strong sharp	1° ≈ 1050 , 2° ≈ 1100 , 3° ≈ 1150 ; phenols ≈ 1220 cm ⁻¹ .
Ethers	Ether C-O C-O-C stretch	1000-1300	Strong sharp	Dialkyl ≈ 1120 . Aryl alkyl ethers show two bands, ≈ 1250 and ≈ 1040 . No O-H or C=O.
Carbonyls	Ketone C=O C=O stretch	1705-1725	Strong sharp	Saturated ketone ≈ 1715 cm ⁻¹ . Conjugation lowers it to 1685-1666. Ring strain raises it (cyclopentanone ≈ 1745 , cyclobutanone ≈ 1780).
Carbonyls	Aldehyde C=O C=O stretch	1720-1740	Strong sharp	Saturated aldehyde ≈ 1725 . Conjugated 1710-1685.
Carbonyls	Aldehyde C-H C-H stretch (Fermi doublet)	2700-2860	Weak-medium sharp	Two peaks near 2820 and 2720 cm ⁻¹ . The 2720 band is diagnostic for an aldehyde.
Carbonyls	Carboxylic acid O-H O-H stretch	2400-3400	Strong very broad	Extremely broad band (H-bonded dimer) that overlaps the C-H stretches.
Carbonyls	Carboxylic acid C=O C=O stretch	1700-1730	Strong sharp	Dimer ≈ 1710 . Conjugated 1710-1680.
Carbonyls	Carboxylic acid C-O C-O stretch	1210-1320	Strong sharp	With the broad O-H and C=O, it confirms a carboxylic acid.
Carbonyls	Ester C=O C=O stretch	1735-1750	Strong sharp	Saturated ester ≈ 1735 . Conjugated or aryl esters 1730-

Class	Functional group / vibration	Wavenumber (cm ⁻¹)	Intensity / shape	Notes
				1715. δ -lactone $\approx$ 1735, γ -lactone $\approx$ 1770.
Carbonyls	Ester C-O C-O stretch	1000-1300	Strong sharp	Two or more strong bands, "rule of three" with the C=O.
Carbonyls	Acid chloride C=O C=O stretch	1775-1810	Strong sharp	$\approx$ 1800 cm ⁻¹ : the highest common single carbonyl.
Carbonyls	Anhydride C=O C=O stretch (asymmetric)	1800-1830	Strong sharp	Anhydrides show two C=O bands about 60 cm ⁻¹ apart.
Carbonyls	Anhydride C=O C=O stretch (symmetric)	1740-1775	Strong sharp	Second anhydride carbonyl band.
Carbonyls	Amide C=O (amide I) C=O stretch	1630-1680	Strong sharp	Lowest common carbonyl, because N lone-pair resonance weakens the C=O.
Amines & amides	Primary amine / amide N-H N-H stretch (two bands)	3300-3500	Medium medium	Two spikes (asymmetric + symmetric). Sharper and weaker than O-H.
Amines & amides	Secondary amine / amide N-H N-H stretch (one band)	3300-3350	Medium medium	One band. Tertiary amines show none.
Amines & amides	Amine N-H bend N-H bend (scissoring)	1560-1640	Medium medium	Primary amines. Amides show the amide II band at 1640-1550.
Amines & amides	Amine C-N C-N stretch	1000-1350	Medium sharp	Aliphatic 1250-1000. Aromatic amines 1350-1250.
Nitrogen groups	Nitrile C$\equiv$N C $\equiv$ N stretch	2210-2260	Medium sharp	Aliphatic $\approx$ 2250. Conjugated or aryl 2240-2220. Sharp and medium.
Nitrogen groups	Isocyanate N=C=O N=C=O asymmetric stretch	2240-2275	Strong broad	Very strong and broad near 2270 cm ⁻¹ .

Class	Functional group / vibration	Wavenumber (cm ⁻¹)	Intensity / shape	Notes
Nitrogen groups	Azide N=N=N N ₃ asymmetric stretch	2120-2160	Strong sharp	Strong band about 2100-2160 cm ⁻¹ .
Nitrogen groups	Imine C=N C=N stretch	1640-1690	Variable sharp	Variable intensity.
Nitrogen groups	Nitro N=O N-O asymmetric stretch	1515-1560	Strong sharp	≈1550. A strong pair with the 1380 band.
Nitrogen groups	Nitro N=O N-O symmetric stretch	1345-1385	Strong sharp	≈1380 cm ⁻¹ .
Sulfur & phosphorus	Thiol S-H S-H stretch	2550-2600	Weak sharp	Weak but in a clear region.
Sulfur & phosphorus	Sulfoxide S=O S=O stretch	1030-1070	Strong sharp	≈1050 cm ⁻¹ .
Sulfur & phosphorus	Sulfone / sulfonyl S=O S=O asymmetric stretch	1300-1350	Strong sharp	Paired with the symmetric band at 1160-1120.
Sulfur & phosphorus	Sulfone / sulfonyl S=O S=O symmetric stretch	1120-1160	Strong sharp	Also seen in sulfonamides and sulfonate esters.
Sulfur & phosphorus	Phosphine P-H P-H stretch	2350-2440	Medium sharp	Sharp, medium.
Sulfur & phosphorus	Phosphoryl P=O P=O stretch	1140-1300	Strong sharp	Phosphates and phosphine oxides.
Halides	C-F C-F stretch	1000-1400	Strong sharp	Very strong. CF ₃ gives several strong bands.
Halides	C-Cl C-Cl stretch	540-785	Strong sharp	Often hidden in the fingerprint region.
Halides	C-Br C-Br stretch	510-650	Strong sharp	Below most mid-IR scans.
Halides	C-I C-I stretch	485-600	Strong sharp	Below most mid-IR scans.
Cumulenes & others	Allene C=C=C C=C=C	1900-1950	Medium sharp	≈1950 cm ⁻¹ .

Class	Functional group / vibration	Wavenumber (cm ⁻¹)	Intensity / shape	Notes
	asymmetric stretch			
Cumulenes & others	Carbon dioxide (artifact) O=C=O asymmetric stretch	2330–2360	Medium sharp	Atmospheric CO ₂ near 2350 cm ⁻¹ : usually a background artifact, not your sample.
Cumulenes & others	Metal carbonyl C≡O C≡O stretch	1800–2100	Strong sharp	Terminal M-CO 2100–1850; bridging 1850–1750.

IUPAC Name to SMILES Converter

<https://www.moldraw.com/tools/free-chem-tools/iupac-name-to-smiles-converter.html>

IUPAC Name to SMILES converter by MolDraw. Convert systematic names to SMILES or import compounds from PubChem by name/CID.

In short: Convert systematic names to SMILES or import compounds from PubChem by name/CID. It is free, works in your web browser and needs no download.

Convert IUPAC names or PubChem compound names to SMILES. Useful for turning literature names into structure strings.

SMILES output appears here.

Input and output formats

Input: IUPAC name	Output: SMILES	
Full name	IUPAC name	SMILES (Simplified Molecular Input Line Entry System)
What it holds	The systematic chemical name made with IUPAC naming rules.	Atoms, bonds, rings, charges and stereo as one line of text. No coordinates.
File or form	Text	.smi or plain text

File Format Explained

IUPAC names are formal chemical names designed to describe structure systematically. They are useful in publications and teaching, but long names can be hard to paste into software workflows.

SMILES is a compact structure string used by drawing tools, databases, cheminformatics scripts, and converters. Converting IUPAC to SMILES helps turn a literature name into a

machine-readable structure.

Name resolution works best for unambiguous, recognized names. Salts, mixtures, stereochemistry, common names, and spelling variations may return no result or a different record.

Tips for name-to-SMILES conversion

Systematic IUPAC names encode a structure precisely, but they are long and easy to mistype. Converting a name to SMILES gives you a compact, machine-readable structure you can paste into drawing tools or spreadsheets.

Examples

- propan-2-ol → CC(C)O
- 2-acetyloxybenzoic acid (aspirin) → CC(=O)OC1=CC=CC=C1C(=O)O
- (2S)-2-aminopropanoic acid (L-alanine) → C[C@@H](C(=O)O)N

Getting good results

- Copy names exactly, including locants, commas, hyphens, and brackets: 1,2-dichloroethane is not the same as 1,1-dichloroethane.
- Include stereodescriptors such as (R), (S), (E), or (Z) if you need a specific isomer; otherwise stereochemistry may be left undefined.
- Common names such as caffeine often work too, but very new or rare trade names may not.
- Watch for typographic characters from PDFs, such as special dashes or primes, and replace them with plain hyphens and apostrophes.

Going the other way? Use [SMILES to IUPAC Name](#).

Related chemistry tools

[CAS Number to SMILES Converter](#)[CID to SMILES Converter](#)[InChI to SMILES Converter](#)[SMILES Notation Guide](#)[SMILES to Structure Converter](#)[Online Structure to SMILES Converter](#)

Lewis Structure Generator - Dot Structures & VSEPR

<https://www.moldraw.com/tools/free-chem-tools/lewis-structure-generator.html>

Free Lewis dot structure generator: enter a formula (SO₄²⁻, NH₃, XeF₄) to get bonds, lone pairs, formal charges and VSEPR shape, with step-by-step help.

In short: Lewis dot structure generator: enter a formula (SO₄²⁻, NH₃, XeF₄) to get bonds, lone pairs, formal charges and VSEPR shape, with step-by-step help. It is free, works in your web browser and needs no download.

Enter a molecule or ion to draw its Lewis dot structure, with bonding pairs, lone pairs and formal charges. You also get the VSEPR geometry and a step-by-step explanation of how the structure was built.

Quick answer: for water, O has 6 valence electrons and each H has 1, giving 8. Two O-H bonds use 4, and the other 4 sit on O as **two lone pairs**, so the molecule is **bent** ($\approx 104.5^\circ$).
Formula Charge

How to use the lewis structure generator

1. Type the formula (NH_4) and choose the charge, or type it with the charge (NO_3^- , SO_4^{2-}).
2. The generator counts valence electrons and picks the central atom (the least electronegative atom, never H).
3. It completes the octets of the outer atoms, places leftover electrons on the central atom, and forms double or triple bonds where the central atom is short of an octet.
4. Read the structure, formal charges, resonance note and VSEPR shape. Download the SVG for worksheets or slides.

Worked examples

Ammonia, NH_3 (8 e^-)

3 N-H bonds (6 e^-) + 1 lone pair on N

Trigonal pyramidal, $\approx 107^\circ$

Carbon dioxide, CO_2 (16 e^-)

$\text{O}=\text{C}=\text{O}$, two lone pairs on each O, formal charges 0

Linear, 180°

Nitrate, NO_3^- (24 e^-)

One $\text{N}=\text{O}$ and two $\text{N}-\text{O}^-$; N is +1, the two single-bonded O are -1

Trigonal planar, 3 resonance structures

Xenon tetrafluoride, XeF_4 (36 e^-)

4 Xe-F bonds + 2 lone pairs on Xe (expanded octet)

Square planar, 90°

How to draw a Lewis structure

1. **Count valence electrons** from the group number (C 4, N 5, O 6, halogens 7). Add one for each negative charge and subtract one for each positive charge.
2. **Draw the skeleton.** The least electronegative atom goes in the centre. H and F are always terminal.
3. **Complete octets on outer atoms** with lone pairs (H only needs 2 electrons).
4. **Put leftover electrons on the central atom.**

5. **Form multiple bonds** if the central atom has fewer than 8 electrons, by turning outer lone pairs into shared pairs.
6. **Check formal charges:** $FC = \text{valence } e^- - \text{lone-pair } e^- - \text{bonds}$. The best structure has charges closest to zero, with any negative charge on the more electronegative atom.

Formal charge = $V - L - B$ (V = valence electrons, L = non-bonding electrons, B = number of bonds)

Exceptions to the octet rule

Incomplete octets: B and Be (BF_3 , BeCl_2). **Expanded octets:** period 3 and heavier atoms (PCl_5 , SF_6 , XeF_4). **Odd-electron radicals:** NO and NO_2 . For sulfate, phosphate and similar ions, the tool shows the formal-charge-minimised structure with $\text{S}=\text{O}$ double bonds. Many textbooks also accept the octet structure with only single bonds and S^{2+} .

VSEPR shapes

Bonded atoms + lone pairs	Shape	Example
2 + 0	Linear	CO_2 , BeCl_2
3 + 0 / 2 + 1	Trigonal planar / bent	BF_3 / SO_2
4 + 0 / 3 + 1 / 2 + 2	Tetrahedral / trigonal pyramidal / bent	CH_4 / NH_3 / H_2O
5 + 0 / 4 + 1 / 3 + 2	Trigonal bipyramidal / seesaw / T-shaped	PCl_5 / SF_4 / ClF_3
6 + 0 / 5 + 1 / 4 + 2	Octahedral / square pyramidal / square planar	SF_6 / BrF_5 / XeF_4

For bond angles, hybridization, polarity and a 3D model of each shape, use the [VSEPR molecular geometry calculator](#).

The generator covers molecules with one central atom, diatomics and X_3^- ions such as I_3^- and O_3 . For larger molecules (ethanol, benzene) draw the skeletal structure in the MolDraw editor.

Drawing bigger molecules? Use the full MolDraw editor for skeletal structures, lone pairs, charges and curved-arrow mechanisms, free in your browser.

[Open MolDraw editor](#)

Frequently asked questions

How do you draw a Lewis structure step by step?

Count valence electrons, put the least electronegative atom in the centre, connect atoms with single bonds, complete the outer octets, put leftover electrons on the centre, then form multiple bonds until the central atom has an octet.

How do you count valence electrons for an ion?

Add the valence electrons of all atoms, then add one electron per negative charge or subtract one per positive charge. SO_4^{2-} has $6 + 4 \times 6 + 2 = 32$.

What is formal charge?

Formal charge = valence electrons – non-bonding electrons – number of bonds. It shows how electrons are distributed; the best Lewis structure keeps formal charges small.

Which atom is the central atom?

Usually the least electronegative atom that is not hydrogen, often the one that appears only once in the formula (S in SO_4^{2-} , C in CO_2 , N in NH_3).

Can atoms have more than 8 electrons?

Yes. Elements in period 3 and below (P, S, Cl, Xe...) can have expanded octets, as in PCl_5 (10 electrons) and SF_6 (12).

What does the Lewis structure tell me about shape?

Counting bonded atoms and lone pairs on the central atom gives the VSEPR shape, for example 3 bonds + 1 lone pair = trigonal pyramidal (NH_3).

Limiting Reagent Calculator - Theoretical Yield

<https://www.moldraw.com/tools/free-chem-tools/limiting-reagent-calculator.html>

Find the limiting reactant, excess left over and theoretical yield from grams, moles or solutions. Auto-balances equations. Free stoichiometry tool.

Set up your stoichiometry calculation

Balanced reaction

Enter the equation with + between species and -> or = as the arrow. If it is not balanced, the calculator balances it for you.

Product of interest

Product Product coefficient Product molar mass (g/mol) Actual yield (optional, g)

Quick presets

Load a reaction and enter reactant amounts to calculate the limiting reagent.

How to Find the Limiting Reagent

1. Make sure the chemical equation is balanced.
2. Convert each reactant amount to moles. For grams, use $\text{moles} = \text{grams} / \text{molar mass}$. For solutions, use $\text{moles} = M \times L$.
3. Divide moles of each reactant by its stoichiometric coefficient.

4. The smallest value is the reaction extent and identifies the limiting reagent.
5. Use the limiting extent to calculate product moles and leftover excess reactants.

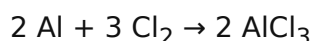
This educational calculator balances the equation if needed and assumes the reaction goes to completion. Real experiments may have side reactions, purity issues, equilibrium limits, or incomplete conversion.

How to use the limiting reagent calculator

1. Type the reaction, e.g. $\text{Al} + \text{Cl}_2 \rightarrow \text{AlCl}_3$, and click *Load reactants*. Unbalanced equations are balanced for you.
2. For each reactant choose grams, moles or solution ($\text{M} \times \text{L}$) and enter the amount. Molar masses are filled in automatically.
3. Pick the product you care about. Add an actual yield to get percent yield.
4. Read the limiting reagent, the leftover excess (mol and g) and the theoretical yield.

Worked examples

10.0 g Al + 50.0 g Cl₂ → AlCl₃

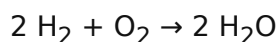


$$\text{Al: } 0.3706 \text{ mol} \div 2 = 0.1853$$

$$\text{Cl}_2: 0.7052 \text{ mol} \div 3 = 0.2351$$

$$\text{Al limits; theoretical yield} = 0.3706 \text{ mol} \times 133.33 = 49.42 \text{ g AlCl}_3$$

4 mol H₂ + 1.5 mol O₂



$$\text{H}_2: 4 \div 2 = 2.0; \text{O}_2: 1.5 \div 1 = 1.5$$

$$\text{O}_2 \text{ limits} \rightarrow 3.0 \text{ mol H}_2\text{O}; 1.0 \text{ mol H}_2 \text{ left over}$$

Writing up the experiment? Draw the reaction scheme with structures and conditions in the free MolDraw reaction drawer.

[Draw the reaction](#)

Frequently asked questions

How do you find the limiting reagent?

Convert each reactant to moles, divide by its coefficient in the balanced equation, and pick the smallest result. That reactant runs out first and sets the amount of product.

Does the equation need to be balanced?

The calculation needs a balanced equation, but you can type an unbalanced one; the calculator balances it automatically and tells you.

How do you calculate theoretical yield?

Multiply the limiting reagent's extent (moles ÷ coefficient) by the product's coefficient to get moles of product, then multiply by the product's molar mass for grams.

How much excess reagent is left over?

Moles used = extent × coefficient. Subtract that from the moles available, and multiply by molar mass for grams. The calculator shows both.

Can I use solution volumes and molarity?

Yes. Choose 'Solution (M × L)' and enter molarity and volume in litres; moles = M × V.

What is percent yield?

Percent yield = actual yield ÷ theoretical yield × 100. Enter your actual mass of product to get it.

Related chemistry tools

Stoichiometry calculator Grams, moles and gas volumes
Theoretical yield calculator Limiting reagent → grams of product
AP Chemistry score calculator Estimate your 1–5 exam score
Chemical equation balancer Balance reactions and redox ions
Percent yield calculator Actual vs theoretical yield
Molar mass calculator Step-by-step molar mass working
Grams to moles calculator Convert mass and moles
Molarity calculator Moles, volume and concentration
Molecular weight calculator Formula to g/mol with % composition
Solution prep calculator Mass needed for a solution
Net ionic equation calculator Complete and net ionic equations

Need to sketch molecules for a report? [Draw chemical structures online](#) with MolDraw, a free online ChemDraw alternative (see the [ChemDraw vs MolDraw comparison](#)).

Lipinski Rule Calculator | Rule of Five Checker

<https://www.moldraw.com/tools/free-chem-tools/lipinski-rule-calculator.html>

Free Lipinski Rule of Five calculator. Enter SMILES or a compound name to check molecular weight, LogP, hydrogen bond donors, and hydrogen bond acceptors.

In short: Enter SMILES or a compound name to check molecular weight, LogP, hydrogen bond donors, and hydrogen bond acceptors. It is free, works in your web browser and needs no download.

Enter a SMILES string or compound name to check the four classic Lipinski Rule of Five properties: molecular weight, LogP, hydrogen-bond donors, and hydrogen-bond acceptors.

Enter a compound to calculate. SMILES Compound name Results appear here.

What Lipinski Rule of Five Means

Lipinski's Rule of Five is a quick oral drug-likeness guideline. A compound is commonly considered more rule-of-five-like when molecular weight is at or below 500, LogP is at or below 5, hydrogen-bond donors are at or below 5, and hydrogen-bond acceptors are at or below 10.

- Rules are screening guidelines, not clinical or biological guarantees.
- Many useful drugs and natural products intentionally violate one or more rules.
- Use the druglikeness calculator for a broader Lipinski plus Veber-style view.

[Druglikeness calculator](#) [LogP calculator](#) [TPSA calculator](#)

Related chemistry tools

[ChEMBL bioactivity plugin](#) [pKa Calculator](#) [SMILES to Molecular Weight Calculator](#) [Mass Spectrum Predictor](#)

LogP Calculator | XLogP from SMILES or Name

<https://www.moldraw.com/tools/free-chem-tools/logp-calculator.html>

Free LogP calculator for SMILES or compound names. Retrieve PubChem XLogP, formula, molecular weight, IUPAC name, and CID.

In short: LogP calculator for SMILES or compound names. It is free, works in your web browser and needs no download.

Enter a SMILES string or compound name to retrieve PubChem XLogP, a hydrophobicity estimate used in medicinal chemistry and formulation screening.

Enter a compound to calculate. SMILES Compound name Results appear here.

What LogP Tells You

LogP estimates the partitioning of a neutral compound between octanol and water. Higher LogP generally means a compound is more hydrophobic; very high values can indicate lower aqueous solubility and possible permeability/formulation tradeoffs.

[Lipinski rule calculator](#) [TPSA calculator](#) [SMILES to molecular weight](#)

Interpreting logP values

logP is the base-10 logarithm of the octanol/water partition coefficient of the neutral form of a compound. A logP of 2 means the compound is about 100 times more concentrated in octanol than in water at equilibrium. XLogP, the value PubChem provides, is a computed estimate based on atom and fragment contributions, not a measurement.

Rough guide

- **Below 0:** hydrophilic. Sugars such as glucose are strongly negative.

- **About 1 to 3:** a common range for orally absorbed drugs.
- **Above 5:** very lipophilic; poor solubility is more likely, and it is one of Lipinski's flags.

logP versus logD

logP describes the neutral molecule only. Acids and bases ionise in water depending on pH, so the measured distribution at a given pH (logD) can be much lower than logP. For a carboxylic acid at pH 7.4, most molecules are ionised, so logD is typically well below logP.

Tip: compare analogues in a series rather than relying on one absolute number; the change in logP when you add a group is often more informative. See also the [Druglikeness Calculator](#).

Related chemistry tools

[pKa Calculator](#)[Mass Spectrum Predictor](#)

Mass Spectrum Predictor | Isotope Pattern Calculator

<https://www.moldraw.com/tools/free-chem-tools/mass-spectrum-predictor.html>

Mass spectrum predictor and isotope pattern tool by MolDraw. Import by PubChem name, draw a molecule, paste SMILES, or enter a formula to estimate monoisotopic mass, average mass, molecular ion peak, M+1/M+2 isotope peaks, and an isotope pattern chart.

In short: Import by PubChem name, draw a molecule, paste SMILES, or enter a formula to estimate monoisotopic mass, average mass, molecular ion peak, M+1/M+2 isotope peaks, and an isotope pattern chart. It is free, works in your web browser and needs no download.

Import a compound by PubChem name, draw a molecule, paste SMILES, or enter a molecular formula to estimate isotope pattern peaks, monoisotopic mass, average mass, and the molecular ion region.

Quick answer: search PubChem by name or CID, draw a structure, paste SMILES, or type a formula. The isotope pattern updates from the molecular formula.

Draw or Paste Input

Import from PubChem by name or CID SMILES input Molecular formula Ready. Formula prediction is fully client-side; SMILES lookup uses PubChem.

Predicted Spectrum

Spectrum chart appears here.

What This Mass Spectrum Tool Predicts

This tool predicts isotope distribution from elemental composition. It is useful for molecular ion peak checks, M+1/M+2 pattern interpretation, chlorine/bromine isotope patterns, and exact mass teaching.

- **Monoisotopic mass:** mass from the lightest common isotopes.

- **Average mass:** abundance-weighted molecular mass.
- **Isotope pattern:** relative molecular ion peaks from natural isotope abundances.

This is not an EI fragmentation or MS/MS predictor. Fragment ions depend on ionization method, collision energy, instrument settings, and molecule-specific fragmentation pathways.

[Exact mass calculator](#) [Molecular weight calculator](#) [Formula to structure search](#) [SMILES to molecular formula](#)

Related chemistry tools

[How to read a mass spectrum](#) [Mass Spectrum Viewer](#) [AI Spectroscopy plugin](#) [Druglikeness Calculator](#) [Lipinski Rule Calculator](#) [TPSA Calculator](#) [LogP Calculator](#) [pKa Calculator](#) [SMILES to Molecular Weight Calculator](#)

MOL to InChI Converter

<https://www.moldraw.com/tools/free-chem-tools/mol-to-inchi-converter.html>

MOL to InChI converter by MolDraw. Convert MOL or SDF structure blocks into standard InChI identifiers for chemistry data workflows.

In short: Convert MOL or SDF structure blocks into standard InChI identifiers for chemistry data workflows. It is free, works in your web browser and needs no download.

Paste a MOL or SDF block and convert it into a standard InChI identifier.

InChI output appears here.

Input and output formats

Input: MOL file	Output: InChI	
Full name	MOL file (MDL Molfile)	InChI (IUPAC International Chemical Identifier)
What it holds	An atom list with 2D or 3D coordinates and a bond table for one molecule.	A layered text identifier built from the structure. The standard InChI is the same in every program.
File or form	.mol	Text starting with InChI=1S/

File Format Explained

MOL stores a molecule as atom and bond tables, often with 2D or 3D coordinates. It is useful for editable structure exchange.

InChI is a standardized text identifier generated from the structure. It is useful for search, indexing, registration, and comparing chemical records across databases.

Conversion quality depends on the MOL file having clear atoms, bonds, charges, and stereochemistry. Review the generated InChI for salts, tautomers, and stereochemical layers.

About MOL files

A MOL file (MDL Molfile) stores a single structure as a connection table: a header, a counts line, an atom block with x, y, z coordinates and element symbols, and a bond block listing which atoms are connected and with what bond order. Most chemistry software can export MOL, which makes it a common exchange format. Two versions exist: V2000, the classic fixed-column format, and V3000, which supports larger molecules and more features.

Why convert to InChI

InChI gives a standard identifier that does not depend on atom order or drawing coordinates. Two MOL files of the same molecule drawn differently produce the same standard InChI, which makes it easy to check for duplicates or search databases.

How to use it

1. Open the .mol file in a text editor and copy everything, including the header lines and the final M END line.
2. Paste it into the input box and convert.
3. Copy the InChI, or shorten it further with [InChI to InChIKey](#).

Troubleshooting: MOL files are column-sensitive, so a file reformatted by a word processor may fail. Copy from a plain-text editor.

Related chemistry tools

[InChIKey to InChI Converter](#)[MOL to InChIKey Converter](#)[MOL to SMILES Converter](#)[SDF to InChI Converter](#)[SMILES Notation Guide](#)[SMILES to Structure Converter Online](#)

MOL to InChIKey Converter

<https://www.moldraw.com/tools/free-chem-tools/mol-to-inchikey-converter.html>

MOL to InChIKey converter by MolDraw. Convert MOL or SDF structure blocks into standard InChIKey identifiers.

In short: Convert MOL or SDF structure blocks into standard InChIKey identifiers. It is free, works in your web browser and needs no download.

Paste a MOL or SDF block and convert it into a standard InChIKey value.

InChIKey output appears here.

Input and output formats

Input: MOL file	Output: InChIKey	
Full name	MOL file (MDL Molfile)	InChIKey
What it holds	An atom list with 2D or 3D coordinates and a bond table for one molecule.	A 27 character hash of the InChI, made for web and database search. It cannot be turned back into a structure without a lookup database.
File or form	.mol	Text like XXXXXXXXXXXXXXXX-YYYYYYYYY-Z

File Format Explained

MOL is a structure file with atom and bond blocks. It can preserve drawn coordinates and editable molecular topology.

InChIKey is a fixed-length key generated from an InChI. It is designed for fast lookup, database matching, and duplicate detection across chemical collections.

Use MOL when you need an editable structure file. Use InChIKey when you need a compact identifier for search or matching.

When an InChIKey is the right output

If you have a structure as a MOL file and want to find it online, register it in a spreadsheet, or check whether two files describe the same compound, an InChIKey is the most practical identifier. It is a fixed-length string, so it fits neatly in a database column and works as a search-engine query.

How to use it

1. Export or open your structure as a .mol file.
2. Copy the full text, from the first header line to M END.
3. Paste and convert, then copy the 27-character key.

Example uses

- **Duplicate checking:** generate keys for a folder of MOL files and sort them; identical keys mean identical structures, even if atoms were numbered differently.
- **Literature search:** search the key in a search engine to find database entries and papers mentioning the compound.
- **Stereo comparison:** compare the first block to see whether two stereoisomers share a skeleton.

Need the full identifier as well? Use [MOL to InChI](#). Have SMILES instead? Use [SMILES to InChIKey](#).

Related chemistry tools

[InChI to InChIKey Converter](#)[MOL to SMILES Converter](#)[SDF to InChIKey Converter](#)[SMILES Notation Guide](#)[SMILES to Structure Converter Online](#)[Structure to SMILES Converter](#)

MOL to SMILES Converter

<https://www.moldraw.com/tools/free-chem-tools/mol-to-smiles-converter.html>

MOL to SMILES converter by MolDraw. Paste MOL/SDF content and convert to SMILES online with a free chemistry tool.

In short: Paste MOL/SDF content and convert to SMILES online. It is free, works in your web browser and needs no download.

Paste, upload, or import a MOL/SDF block from PubChem, then convert it to SMILES. This tool attempts PubChem conversion first, then falls back to NCI Cactus when possible.

Upload .mol or .sdf file

Paste MOL/SDF content, upload a file, or import a 2D SDF record from PubChem.

SMILES output appears here.

Input and output formats

Input: MOL file	Output: SMILES	
Full name	MOL file (MDL Molfile)	SMILES (Simplified Molecular Input Line Entry System)
What it holds	An atom list with 2D or 3D coordinates and a bond table for one molecule.	Atoms, bonds, rings, charges and stereo as one line of text. No coordinates.
File or form	.mol	.smi or plain text

File Format Explained

MOL and **SDF** files store atom and bond blocks, often with 2D or 3D coordinates. They are useful for editable structure exchange and compound data records.

SMILES converts that structure into a compact one-line text notation. It is useful for search, identifiers, scripts, and web tools.

When converting MOL or SDF to SMILES, check stereochemistry, charges, salts, and aromaticity. Some coordinate or property data from the source file will not be preserved in SMILES.

Related chemistry tools

[SMILES to MOL Converter](#)[CAS Number to SMILES Converter](#)[CID to SMILES Converter](#)[InChI to SMILES Converter](#)[SMILES Notation Guide](#)[SMILES to Structure Converter Online](#)