

MolDraw free tools (part 2)

The rest 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

MOL2 to SMILES Converter

<https://www.moldraw.com/tools/free-chem-tools/mol2-to-smiles-converter.html>

MOL2 to SMILES converter by MolDraw. Convert MOL2 text to SMILES using a best-effort public resolver workflow.

In short: Convert MOL2 text to SMILES using a best-effort public resolver workflow. It is free, works in your web browser and needs no download.

Convert MOL2 content to SMILES. Best for smaller ligand MOL2 blocks.

SMILES output appears here.

Input and output formats

Input: MOL2	Output: SMILES	
Full name	MOL2 (Tripos Mol2)	SMILES (Simplified Molecular Input Line Entry System)
What it holds	3D coordinates, bonds, atom types and partial charges.	Atoms, bonds, rings, charges and stereo as one line of text. No coordinates.
File or form	.mol2	.smi or plain text

File Format Explained

MOL2 is a Tripos structure format used in docking and modeling. It can include atom coordinates, atom types, substructure records, bonds, and charge values.

SMILES is a one-line molecular identifier focused on connectivity. Converting MOL2 to SMILES is useful when you need a searchable string for a ligand from a modeling workflow.

MOL2 files can contain atom-type and charge information that SMILES will not preserve. Check stereochemistry and protonation after conversion.

About MOL2 files

The Tripos MOL2 format is common in molecular modelling and docking. Unlike a MOL file, it stores SYBYL atom types (such as C.ar for aromatic carbon or N.am for amide nitrogen), partial charges, and substructure information in sections that start with tags like @<TRIPOS>MOLECULE, @<TRIPOS>ATOM, and @<TRIPOS>BOND. Docking programs and ligand libraries often supply molecules in MOL2.

Why convert to SMILES

SMILES is far easier to read, store, and search. Converting a docked ligand or library entry to SMILES lets you check its identity, paste it into a spreadsheet, or redraw it for a figure.

How to use it

1. Open the .mol2 file in a text editor and copy one molecule, from @<TRIP0S>MOLECULE through the bond section.
2. Paste and convert.
3. Check the SMILES by drawing it with [SMILES to Structure](#).

Watch out: files prepared for docking often include explicit hydrogens and a specific protonation state, so the SMILES may show charged groups such as a protonated amine.

Related chemistry tools

[SMILES to MOL2 Converter](#)[CAS Number to SMILES Converter](#)[CID to SMILES Converter](#)[InChI to SMILES Converter](#)[SMILES Notation Guide](#)[Structure to SMILES Converter](#)

Molality Calculator

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

Free molality calculator for chemists. Compute molality from solute mass, molecular weight, and solvent mass.

In short: Compute molality from solute mass, molecular weight, and solvent mass. It is free, works in your web browser and needs no download.

Compute solution molality from solute mass, molecular weight, and solvent mass.

Solute mass (g) Molecular weight (g/mol) Solvent mass (g) Enter valid values.

How molality is calculated

Molality (m) is moles of solute per kilogram of solvent: **$m = (\text{mass in g} \div \text{molecular weight in g/mol}) \div \text{solvent mass in kg}$** . Example: 1.50 g of NaCl (58.44 g/mol) in 100 g of water gives $0.02567 \text{ mol} \div 0.100 \text{ kg} = 0.257 \text{ mol/kg}$.

Because it uses mass rather than volume, molality does not change with temperature. It is the unit used for colligative properties such as boiling point elevation and freezing point depression.

Example use: the freezing-point depression of a solution is $\Delta T = i \times K_f \times m$, where K_f for water is $1.86 \text{ }^\circ\text{C}\cdot\text{kg/mol}$ and i is the van 't Hoff factor (about 2 for NaCl). A 0.257 mol/kg NaCl solution therefore freezes roughly $0.96 \text{ }^\circ\text{C}$ below pure water, ignoring non-ideal behaviour. Weigh the solvent rather than measuring its volume.

Molar Mass Calculator - Step-by-Step Working

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

Molar mass calculator with step-by-step working. Learn how to calculate molar mass of any compound in g/mol, then convert grams to moles. Free.

In short: Molar mass calculator with step-by-step working. It is free, works in your web browser and needs no download.

Enter a compound to see its molar mass in g/mol and every step of the calculation, the way you would write it in an exam. Add a mass to convert grams to moles in the same place.

Quick answer: to calculate molar mass, multiply each element's atomic mass by its subscript and add them. $\text{NaCl} = 22.990 + 35.45 = \mathbf{58.440 \text{ g/mol}}$. Compound formula Mass in grams (optional, for grams $\rightarrow$ moles) Enter a formula.

How to use the molar mass calculator

1. Write the correct chemical formula (for example H_2SO_4).
2. Look up the atomic mass of each element on the [periodic table](#). The calculator does this for you.
3. Multiply each atomic mass by how many of that atom are in the formula. Remember that a subscript after a bracket multiplies everything inside it.
4. Add the values. The total is the molar mass in g/mol. Enter a mass to convert grams to moles with $n = m / M$.

Worked examples

Sulfuric acid, H_2SO_4

$$\text{H: } 2 \times 1.008 = 2.016$$

$$\text{S: } 1 \times 32.06 = 32.060$$

$$\text{O: } 4 \times 15.999 = 63.996$$

$$M = 98.072 \text{ g/mol}$$

Calcium carbonate, CaCO_3

$$40.078 + 12.011 + 3 \times 15.999$$

$$M = 100.086 \text{ g/mol}$$

$$\text{So } 25.0 \text{ g CaCO}_3 = 25.0 \div 100.086 = 0.2498 \text{ mol.}$$

Carbon dioxide, CO_2

$$12.011 + 2 \times 15.999$$

$$M = 44.009 \text{ g/mol}$$

How to calculate molar mass

Molar mass (M) is the mass of one mole (6.022×10^{23} particles) of a substance. Its units are grams per mole. Because the atomic mass unit is defined so that one mole of atoms of mass 1 u weighs 1 g, the molar mass in g/mol equals the relative formula mass.

$$M = \sum (\text{subscript} \times \text{atomic mass}) \quad n = m / M \quad m = n \times M$$

Tips that avoid common mistakes

- **Brackets multiply.** In $\text{Mg}_3(\text{PO}_4)_2$ there are 2 P and 8 O atoms, so $M = 3(24.305) + 2(30.974) + 8(15.999) = 262.855 \text{ g/mol}$.
- **Diatomic elements.** Oxygen gas is O_2 (31.998 g/mol), not O (15.999 g/mol).
- **Hydrates** include the water: $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$ is 249.677 g/mol, while anhydrous CuSO_4 is 159.602 g/mol.
- **Rounding.** Keep at least 3 decimal places until the final answer, then round to your data's significant figures.

Why is the molar mass of H_2O 18?

Two hydrogen atoms ($2 \times 1.008 = 2.016$) plus one oxygen (15.999) give 18.015 g/mol, which rounds to 18. One mole of water weighs about 18 g, and 18 mL of liquid water at room temperature is roughly one mole.

For a full element-by-element percent composition table use the [molecular weight calculator](#).

Working from a structure? Sketch it in MolDraw and the editor shows the molecular formula and molar mass as you draw.

[Draw it in MolDraw](#)

Frequently asked questions

How do you calculate molar mass?

Multiply each element's atomic mass by the number of times it appears in the formula, then add all the values. The answer is in g/mol.

What is the formula for calculating molar mass?

$M = \sum(n \times A)$, where n is the number of atoms of each element and A is its atomic mass. To link mass and moles use $n = m / M$.

What is the molar mass of water?

18.015 g/mol ($2 \times 1.008 + 15.999$).

How do I find molar mass without knowing the compound?

Measure a mass and the number of moles (for a gas, from $PV = nRT$; for a solution, from a titration) and divide: $M = m / n$.

What is the molar mass of 4 H₂O?

The molar mass of H₂O is still 18.015 g/mol. '4 H₂O' means four moles (or molecules), which have a mass of $4 \times 18.015 = 72.06$ g.

What is the difference between molar mass and molecular weight?

They have the same numerical value. Molar mass carries units of g/mol; molecular weight is a dimensionless relative mass.

Related chemistry tools

Stoichiometry calculator Grams, moles and gas volumes **Ideal gas law calculator** $PV = nRT$ and gas laws **Molecular weight calculator** Formula to g/mol with % composition **Grams to moles calculator** Convert mass and moles **Empirical formula calculator** Percent composition to formula **Molarity calculator** Moles, volume and concentration **Limiting reagent calculator** Limiting reactant and theoretical yield **Percent yield calculator** Actual vs theoretical yield **Interactive periodic table** All 118 elements with data **Chemical equation balancer** Balance reactions and redox ions

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

Molarity Calculator

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

Free molarity calculator for chemists. Compute molarity from mass, molecular weight, and solution volume.

In short: Compute molarity from mass, molecular weight, and solution volume. It is free, works in your web browser and needs no download.

Compute solution molarity from solute mass, molecular weight, and final solution volume.

Solute mass (g) Molecular weight (g/mol) Final volume (mL) Enter valid values.

How molarity is calculated

Molarity (M) is moles of solute per litre of solution: **$M = (\text{mass in g} \div \text{molecular weight in g/mol}) \div \text{volume in L}$** . The calculator converts your volume from mL to L for you. Example: 1.50 g of NaCl (58.44 g/mol) in 250 mL gives $0.02567 \text{ mol} \div 0.250 \text{ L} = 0.103 \text{ M}$.

Use the final volume of the whole solution, not the volume of solvent added. Molarity changes slightly with temperature because volume does; if you need a temperature-independent value, use molality instead.

Molarity versus molality: molarity divides by litres of solution, molality by kilograms of solvent. For dilute aqueous solutions near room temperature the two numbers are close, but they diverge for concentrated solutions or other solvents. **Units:** $1 \text{ M} = 1 \text{ mol/L} = 1000 \text{ mM}$. To dilute a stock you have made, continue with the dilution calculator.

Related chemistry tools

[Half-Life Calculator](#)[Ideal Gas Law Calculator \(PV = nRT\)](#)[Stoichiometry Calculator](#)

Molecular Formula Finder - From Exact Mass (ppm) or Elemental Analysis

<https://www.moldraw.com/tools/free-chem-tools/molecular-formula-finder.html>

Find molecular formulas from an accurate mass (HRMS, $[M+H]^+$, $[M+Na]^+$, ppm tolerance, element limits, nitrogen rule, RDBE) or from CHN elemental analysis plus molar mass. Free, ranked by error.

In short: Find molecular formulas from an accurate mass (HRMS, $[M+H]^+$, $[M+Na]^+$, ppm tolerance, element limits, nitrogen rule, RDBE) or from CHN elemental analysis plus molar mass. It is free, works in your web browser and needs no download.

Turn a high-resolution mass spectrum peak or a CHN elemental analysis into candidate molecular formulas. Set the ion type, ppm tolerance and element ranges. Every candidate is checked against the RDBE and nitrogen rules and ranked by error.

Quick answer: m/z 195.0877 as $[M+H]^+$ (5 ppm, CHNO) gives **C₈H₁₀N₄O₂** (caffeine). Elemental analysis C 40.00%, H 6.71% with M $\approx$ 180 gives **C₆H₁₂O₆**. Measured m/z/ion type Tolerance (ppm)

Element ranges (min-max atoms)

RDBE $\geq$ 0 H/C 0.2–3.1 (plausible) Approx. molar mass (g/mol) Mass window ($\pm\%$) % tolerance ($\pm$) Oxygen = 100% – rest

How the formula finder works

From an accurate mass

1. **Convert the ion to the neutral mass.** Subtract the adduct: a proton (1.007276 Da) for $[M+H]^+$, Na⁺ (22.989221 Da) for $[M+Na]^+$. Add a proton back for $[M-H]^-$.
2. **Enumerate formulas** inside your element ranges whose monoisotopic mass (¹²C = 12.000000, ¹H = 1.007825, ¹⁴N = 14.003074, ¹⁶O = 15.994915 Da...) lies within the ppm window: error (ppm) = (calculated – measured) $\div$ measured $\times 10^6$.
3. **Apply chemical rules.** The ring-plus-double-bond equivalent (RDBE = C – H/2 – X/2 + N/2 + 1) must be a whole number ≥ 0 for a neutral, even-electron molecule. That automatically enforces the **nitrogen rule**: an odd nominal mass means an odd number of N atoms. An H/C ratio between 0.2 and 3.1 removes formulas that are possible on paper but chemically implausible.
4. **Rank by mass error.** At 5 ppm a small molecule usually has only a handful of candidates. Isotope patterns (Cl, Br, S) and fragments narrow them further.

From elemental (CHN) analysis

Combustion analysis gives mass percentages of C, H and N (and sometimes S or halogens). Oxygen is usually taken by difference. With an approximate molar mass, for example from MS, the finder tries every formula in the mass window and keeps those whose calculated percentages all agree within $\pm 0.4\%$, the usual journal acceptance limit. If you only want the simplest whole-number ratio from percentages, use the [empirical formula calculator](#).

Worked example

An ESI-MS peak at **m/z 195.0877** as $[M+H]^+$ gives $M = 194.0804$ Da. Searching C, H, N and O within 5 ppm gives **C₈H₁₀N₄O₂** (caffeine, calculated $[M+H]^+$ 195.08765, error ≈ -0.3 ppm, RDBE 6). The even nominal mass (194) fits the even N count (4).

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 find a molecular formula from an exact mass?

Enter the measured m/z, pick the ion type ($[M+H]^+$, $[M+Na]^+$, $[M-H]^-$...) and a ppm tolerance. The finder subtracts the adduct, lists every formula within your element limits that matches to within that ppm, and removes those that break the RDBE and nitrogen rules.

What ppm tolerance should I use?

Use 5 ppm for typical Orbitrap or Q-TOF data, or 2–3 ppm for well-calibrated instruments. Low-resolution instruments need 20 ppm or more and give many more candidates.

What is the nitrogen rule?

A neutral organic molecule with an odd nominal mass contains an odd number of nitrogen atoms. One with an even nominal mass has zero or an even number of N.

What is RDBE?

Ring plus double bond equivalents, the same as the degree of unsaturation: $C - H/2 - X/2 + N/2 + 1$. A neutral, closed-shell molecule must have a whole-number RDBE of 0 or more.

How is this different from the empirical formula calculator?

The empirical formula calculator converts exact percentages into the simplest whole-number ratio. This finder searches for whole molecular formulas that fit measured data within experimental error, either from HRMS mass or from CHN analysis plus a molar mass, and ranks them.

Why does the finder return several formulas?

Different formulas can have almost the same mass, especially above about 300 Da. Use a tighter ppm window, sensible element ranges, isotope patterns (Cl and Br are distinctive) and other data to decide.

Related chemistry tools

How to read an NMR spectrum Solve structures **How to read a mass spectrum** M^+ , isotopes **Exact mass calculator** Formula $\rightarrow$ monoisotopic mass **Empirical formula calculator** % composition $\rightarrow$ formula **Degree of unsaturation** RDBE / IHD **Formula to structure** Candidate compounds **IR spectroscopy chart** Functional groups **Molar mass calculator** Average molar mass

Molecular Formula to Structure Search | Formula to Molecule

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

Molecular formula to structure search by MolDraw. Enter a formula such as C₉H₈O₄ and browse matching PubChem structures, names, SMILES, formula, MW, and CID.

In short: Enter a formula such as C₉H₈O₄ and browse matching PubChem structures, names, SMILES, formula, MW, and CID. It is free, works in your web browser and needs no download.

Enter a formula such as C₉H₈O₄ or C₆H₁₂O₆ to browse multiple possible PubChem structure matches. Formula searches are often ambiguous, so this page shows candidate molecules instead of pretending there is only one structure.

Quick answer: formula-to-structure lookup returns candidate compounds with structure image, name, SMILES, formula, molecular weight, and CID. Molecular formula Candidate structures appear below.

Why Formula Searches Return Multiple Structures

A molecular formula only tells you atom counts. Many compounds can share the same formula but have different connectivity, stereochemistry, or functional groups. Use the candidate names, images, and SMILES to choose the intended molecule.

[Name to Structure](#) [SMILES to Structure](#) [Exact Mass Calculator](#)

Why one formula has many structures

A molecular formula only counts atoms; it says nothing about how they are connected. Different compounds with the same formula are isomers. C₂H₆O is both ethanol (an alcohol) and dimethyl ether, two compounds with very different boiling points. Larger formulas can correspond to thousands of known compounds, which is why this tool shows a list of candidates rather than a single answer.

Narrowing down the candidates

- **Degree of unsaturation:** for $C_cH_hN_nX_x$, $DoU = (2c + 2 + n - h - x) \div 2$. Each ring or π bond counts as one. C_6H_6 gives 4, consistent with benzene's ring plus three double bonds.
- **Spectroscopy:** IR shows functional groups, and NMR shows how many distinct environments are present.
- **Context:** the reaction you ran or the source of the sample often rules out most candidates.

Example: $C_9H_8O_4$ returns aspirin among other matches; check the CID and structure before you use one. If you already know the name, [Name to Structure](#) is faster.

Related chemistry tools

[CAS Number to Structure](#)[SMILES Notation Guide](#)[Structure to SMILES Converter](#)[IUPAC Name to SMILES Converter](#)[Molecular Formula Finder](#)[Empirical Formula Calculator](#)[Build a Molecule](#)[Degree of Unsaturation Calculator](#)[IR Spectroscopy Chart \(Correlation Table\)](#)

Molecular Weight Calculator - Free, Instant

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

Free molecular weight calculator: type any formula ($CuSO_4 \cdot 5H_2O$, $Ca(OH)_2$) and get g/mol, element breakdown and % composition instantly. Try it now.

In short: Molecular weight calculator: type any formula ($CuSO_4 \cdot 5H_2O$, $Ca(OH)_2$) and get g/mol, element breakdown and % composition instantly. It is free, works in your web browser and needs no download.

Type a chemical formula and get its molecular weight (molar mass) in g/mol, with a per-element breakdown and percent composition. Works with parentheses, brackets, hydrates and all 118 elements.

Quick answer: molecular weight = sum of (number of atoms $\times$ atomic weight) for every element. For example, $H_2O = 2 \times 1.008 + 15.999 = \mathbf{18.015 \text{ g/mol}}$. Chemical formula

Try an example

Hydrates: use $\cdot$, $*$ or a dot ($CuSO_4 \cdot 5H_2O$). Element symbols are case-sensitive: Co is cobalt, CO is carbon monoxide.

Enter a formula to calculate molecular weight.

How to use the molecular weight calculator

1. Type the chemical formula, for example $Ca(OH)_2$ or $C_6H_{12}O_6$. Use correct capitalisation for element symbols.
2. Use parentheses or brackets for groups ($Al_2(SO_4)_3$, $K_4[Fe(CN)_6]$) and a dot or $\cdot$ for hydrates ($CuSO_4 \cdot 5H_2O$).

3. Read the molecular weight in g/mol. The table shows the atoms of each element, their mass contribution and mass percent.
4. Click *Copy result* to paste the answer into your notes, or open a related tool to convert grams to moles.

Worked examples

Water, H₂O

$$2 \times 1.008 + 1 \times 15.999$$

$$= 18.015 \text{ g/mol}$$

Glucose, C₆H₁₂O₆

$$6 \times 12.011 + 12 \times 1.008 + 6 \times 15.999$$

$$= 72.066 + 12.096 + 95.994$$

$$= 180.156 \text{ g/mol}$$

Copper(II) sulfate pentahydrate, CuSO₄·5H₂O

$$\text{CuSO}_4 (159.60) + 5 \times \text{H}_2\text{O} (18.015)$$

$$= 249.677 \text{ g/mol}$$

Molecular weight formula

The molecular weight (MW) of a substance is the mass of one mole of it, in grams per mole (g/mol). It is found by adding the standard atomic weights of all the atoms in the formula:

$\text{MW} = \sum (n_i \times A_i)$ where n_i = number of atoms of element i , A_i = standard atomic weight

Atomic weights come from the IUPAC table of standard atomic weights (abridged values, e.g. C = 12.011, H = 1.008, O = 15.999, N = 14.007). For elements with no stable isotope (Tc, Pm and everything from Po onwards) the mass number of the longest-lived isotope is used, as on most periodic tables.

Molecular weight vs molar mass vs formula weight

In everyday chemistry the three terms give the same number. **Molar mass** has units of g/mol. **Molecular weight** (relative molecular mass, M_r) is strictly unitless but numerically equal. **Formula weight** is used for ionic compounds such as NaCl that do not form discrete molecules. For mass spectrometry you usually want the [monoisotopic exact mass](#) instead.

Percent composition

Each element's mass percent is its mass contribution divided by the molecular weight $\times 100$. In glucose, carbon contributes $72.066 / 180.156 = 40.00\%$ of the mass. Going the other way, from percentages to a formula, is what the [empirical formula calculator](#) does.

Have a structure rather than a formula? Draw it in the free MolDraw editor and get the formula, molecular weight and exact mass automatically.

[Open MolDraw editor](#)

Frequently asked questions

How do you calculate molecular weight?

Multiply the number of atoms of each element by its atomic weight and add the results. For CO₂: $12.011 + 2 \times 15.999 = 44.009$ g/mol.

What is the molecular weight of water (H₂O)?

18.015 g/mol: two hydrogen atoms ($2 \times 1.008 = 2.016$) plus one oxygen atom (15.999). It is often rounded to 18 g/mol.

Is molecular weight the same as molar mass?

Numerically yes. Molar mass is expressed in g/mol, while molecular weight (relative molecular mass) is a unitless ratio with the same value.

How do I enter hydrates or complex ions?

Use a dot, asterisk or middle dot for water of crystallisation (CuSO₄.5H₂O) and brackets or parentheses for groups (K₄[Fe(CN)₆], Ca₃(PO₄)₂).

Why does my formula say unknown element?

Element symbols are case-sensitive. Write Co for cobalt, Cl for chlorine and Mg for magnesium; CO and CL are read as carbon + oxygen and an invalid symbol.

How do I find the molecular weight of a protein?

Use the protein molecular weight calculator, which sums amino-acid residue masses from a one-letter sequence and adds one water.

Related chemistry tools

Molar mass calculator Step-by-step molar mass working
Empirical formula calculator Percent composition to formula
Grams to moles calculator Convert mass and moles
Exact mass calculator Monoisotopic mass for MS
Protein molecular weight calculator Sequence to kDa and extinction coefficient
SMILES to molecular weight MW straight from a SMILES string
Molarity calculator Moles, volume and concentration
Limiting reagent calculator Limiting reactant and theoretical yield

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

Name to Structure Tool | Chemical Name to Molecule

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

Chemical name to structure tool by MolDraw. Enter a compound name and get the structure image, SMILES, formula, molecular weight, IUPAC name, and PubChem CID.

In short: Enter a compound name and get the structure image, SMILES, formula, molecular weight, IUPAC name, and PubChem CID. It is free, works in your web browser and needs no download.

Enter a chemical name, common name, or IUPAC name to retrieve the matching structure image, SMILES, formula, molecular weight, and PubChem CID.

Quick answer: search names like aspirin, caffeine, ibuprofen, glucose, or ethanol to view the molecule structure. Chemical or compound name [Open in MolDraw](#) Structure metadata appears here. Structure image appears here.

How Name to Structure Lookup Works

The tool resolves names through PubChem and then displays a 2D structure image with key metadata. Always verify salts, mixtures, stereochemistry, and ambiguous common names before using the result in publication or modeling workflows.

[Structure to SMILES](#) [SMILES to Structure](#) [Formula to Structure](#)

Which names work

The lookup accepts common names (caffeine, aspirin), systematic IUPAC names (1,3,7-trimethylpurine-2,6-dione), and many synonyms recorded in PubChem, including some trade names and abbreviations. The result shows the structure, SMILES, formula, molecular weight, and CID so you can confirm you found the right compound.

Avoiding the wrong match

- **Ambiguous names:** "xylene" can mean the ortho, meta, or para isomer, or a mixture. Use o-xylene or 1,2-dimethylbenzene to be specific.
- **Salts:** "metformin hydrochloride" and "metformin" are different records; choose the one that matches your sample.
- **Stereoisomers:** include (R)/(S) or D/L when it matters, for example L-alanine rather than alanine.
- **Spelling:** British and American spellings (sulphate/sulfate, aluminium/aluminum) usually both work, but typos will not.

Next steps: click [Open in MolDraw](#) to edit the structure, or copy the SMILES into converters such as [SMILES to MOL](#). For candidates matching a formula, use [Molecular Formula to Structure](#).

Related chemistry tools

[CAS Number to Structure](#)[SMILES Notation Guide](#)[IUPAC Name to SMILES Converter](#)[Draw a chemical reaction in your browser](#)[TLC Diagram Tool](#)[Chemical Equation Balancer](#)[3D Molecular Model Viewer](#)

Net Ionic Equation Calculator - Spectator Ions

<https://www.moldraw.com/tools/free-chem-tools/net-ionic-equation-calculator.html>

Free net ionic equation calculator: balances the molecular equation, writes the complete ionic equation and cancels spectator ions using solubility rules.

In short: Net ionic equation calculator: balances the molecular equation, writes the complete ionic equation and cancels spectator ions using solubility rules. It is free, works in your web browser and needs no download.

Enter a molecular equation, for example a precipitation or neutralisation reaction. The calculator balances it, splits strong electrolytes into ions using the solubility rules, and cancels the spectator ions to leave the net ionic equation.

Quick answer: for $\text{AgNO}_3 + \text{NaCl} \rightarrow \text{AgCl} + \text{NaNO}_3$ the net ionic equation is **$\text{Ag}^+(\text{aq}) + \text{Cl}^-(\text{aq}) \rightarrow \text{AgCl}(\text{s})$** . Na^+ and NO_3^- are spectator ions. Molecular equation (balanced or unbalanced) Results appear here.

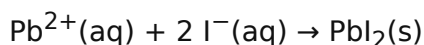
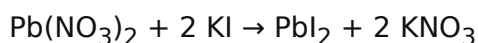
Add states such as $\text{CaCO}_3(\text{s})$ to override the solubility rules. Only common inorganic acids, bases and salts are recognised. Check unusual compounds yourself.

How to use the net ionic equation calculator

1. Enter the molecular equation with ordinary formulas: $\text{BaCl}_2 + \text{Na}_2\text{SO}_4 = \text{BaSO}_4 + \text{NaCl}$. It does not need to be balanced.
2. The tool balances it, then decides for each compound whether it dissolves as ions (strong acids, strong bases, soluble salts) or stays together (precipitates, gases, water, weak acids, metals).
3. It writes the complete ionic equation and cancels ions that appear unchanged on both sides (the spectator ions).
4. Read the net ionic equation. Expand *Why each species was split* to see which solubility rule was applied.

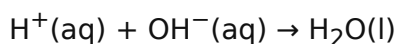
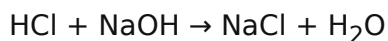
Worked examples

Precipitation: lead(II) iodide

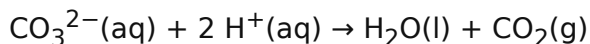
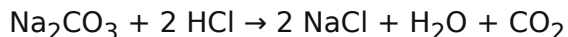


Spectators: K^+ , NO_3^-

Neutralisation



Gas-forming: carbonate + acid



Molecular, complete ionic and net ionic equations

A **molecular equation** shows complete formulas. The **complete ionic equation** writes every strong electrolyte dissolved in water as separate ions. Ions that appear unchanged on both sides are **spectator ions**. Removing them leaves the **net ionic equation**, which shows the chemistry that actually happens.

Solubility rules used

Usually soluble (split into ions)	Exceptions (stay solid)
Group 1 (Li^+ , Na^+ , K^+ ...) and NH_4^+ salts	none
Nitrates, acetates, perchlorates, chlorates	none
Chlorides, bromides, iodides	Ag^+ , Pb^{2+} , Hg_2^{2+} , Cu^+
Sulfates	Ba^{2+} , Sr^{2+} , Pb^{2+} , Ca^{2+} , Ag^+ , Hg_2^{2+}
Usually insoluble (stay solid)	Exceptions (soluble)
Hydroxides	Group 1, Ba^{2+} , Sr^{2+} , Ca^{2+} (moderately)
Carbonates, phosphates, sulfides, sulfites, chromates, oxalates, oxides	Group 1 and NH_4^+

Strong acids (HCl , HBr , HI , HNO_3 , H_2SO_4 , HClO_4 , HClO_3) are split into ions. Weak acids such as CH_3COOH and HF , plus water, gases and metals, stay as written.

Limitations. The rules are the standard general-chemistry simplifications. Slightly soluble salts (CaSO_4 , $\text{Ca}(\text{OH})_2$), H_2SO_4 's second dissociation, complex ions and organic salts are simplified. If you know a state, type it (e.g. $\text{CaSO}_4(\text{aq})$) and the tool will follow it.

Teaching precipitation reactions? Draw apparatus and reaction schemes for worksheets in the MolDraw editor, which is free to use.

[Open MolDraw editor](#)

Frequently asked questions

How do you write a net ionic equation?

Balance the molecular equation, split all soluble strong electrolytes into ions, then cancel ions that appear unchanged on both sides. What remains is the net ionic equation.

What are spectator ions?

Ions that are present in the solution but do not take part in the reaction. They appear identically on both sides of the complete ionic equation, for example Na^+ and NO_3^- in $\text{AgNO}_3 + \text{NaCl}$.

Which compounds are split into ions?

Strong acids, strong bases and soluble ionic salts in aqueous solution. Solids (precipitates), liquids such as water, gases, weak acids and weak bases, and metals are kept as complete formulas.

What if there is no net ionic equation?

If every ion is a spectator, for example $\text{NaCl} + \text{KNO}_3$, no precipitate, gas or water forms and there is no net reaction.

Is the net ionic equation for every strong acid + strong base the same?

Yes. For any strong acid with a strong hydroxide base that forms a soluble salt, the net ionic equation is $\text{H}^+(\text{aq}) + \text{OH}^-(\text{aq}) \rightarrow \text{H}_2\text{O}(\text{l})$.

Does the calculator know every compound's solubility?

No. It applies the standard solubility rules for common ions and flags compounds it is unsure about. Add a state symbol to override it.

Related chemistry tools

Chemical equation balancer Balance reactions and redox ions
Oxidation number calculator Oxidation states with steps
Molarity calculator Moles, volume and concentration
Limiting reagent calculator Limiting reactant and theoretical yield
pH calculator pH, pOH, weak acids and buffers
Molar mass calculator Step-by-step molar mass working
Dilution calculator $C_1V_1 = C_2V_2$ dilutions
Percent yield calculator Actual vs theoretical yield

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

Oxidation Number Calculator - With Steps

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

Find the oxidation number of every element in a compound or ion ($\text{K}_2\text{Cr}_2\text{O}_7$, MnO_4^- , H_2O_2) with step-by-step rules. Free oxidation state calculator.

In short: Find the oxidation number of every element in a compound or ion ($\text{K}_2\text{Cr}_2\text{O}_7$, MnO_4^- , H_2O_2) with step-by-step rules. It is free, works in your web browser and needs no download.

Enter a formula or ion to get the oxidation state of each element, with the rule used at every step. It handles peroxides, metal hydrides, OF₂, polyatomic ions and fractional (average) oxidation states.

Quick answer: in K₂Cr₂O₇, K = +1 and O = -2, so 2(+1) + 2x + 7(-2) = 0 and **Cr = +6**.

Formula or ion

Write ion charges at the end: SO₄²⁻, NH₄⁺, Fe³⁺.

Results appear here.

How to use the oxidation number calculator

1. Type a neutral formula (KMnO₄) or an ion with its charge (Cr₂O₇²⁻, NH₄⁺).
2. The calculator applies the oxidation-number rules in priority order: F, then Group 1, Group 2, Al, H, O and the halogens.
3. The element with no fixed rule is found by making the sum of oxidation numbers equal the overall charge.
4. Read the table and the numbered steps. Fractional answers are averages over atoms in different environments.

Worked examples

Potassium permanganate, KMnO₄

$$K = +1, O = -2$$

$$(+1) + x + 4(-2) = 0$$

$$Mn = +7$$

Hydrogen peroxide, H₂O₂

$$H = +1, \text{ so } 2(+1) + 2x = 0$$

$$O = -1 \text{ (peroxide)}$$

Dichromate ion, Cr₂O₇²⁻

$$O = -2, \text{ total charge } -2$$

$$2x + 7(-2) = -2$$

$$Cr = +6$$

Magnetite, Fe₃O₄

$$3x + 4(-2) = 0$$

$$Fe = +8/3 \text{ (average of one Fe}^{2+} \text{ and two Fe}^{3+}\text{)}$$

Rules for assigning oxidation numbers

1. An atom in an element (Na, O₂, S₈) is 0.
2. A monatomic ion equals its charge (Fe³⁺ = +3, Cl⁻ = -1).
3. Fluorine is always -1 in compounds.
4. Group 1 metals are +1, Group 2 metals are +2 and aluminium is +3.
5. Hydrogen is +1 with non-metals and -1 in metal hydrides (NaH, CaH₂, LiAlH₄).
6. Oxygen is -2, except in peroxides (-1), superoxides (-½) and OF₂ (+2).
7. Cl, Br and I are -1 unless bonded to oxygen or a more electronegative halogen.
8. The sum of all oxidation numbers equals the overall charge: 0 for a compound, the ion charge for an ion.

The calculator follows these rules in that order, which is how exceptions such as peroxides fall out naturally: in H₂O₂ hydrogen is fixed first, so oxygen has to be -1 to make the sum zero.

Oxidation, reduction and identifying Fe²⁺ vs Fe³⁺

An increase in oxidation number is oxidation; a decrease is reduction (OIL RIG). To tell whether iron is +2 or +3 in a compound, balance the charges of the other ions: in FeCl₃, three Cl⁻ means Fe³⁺; in FeSO₄, SO₄²⁻ means Fe²⁺. Going from Fe²⁺ to Fe³⁺ is oxidation.

Limitations. Rules give one value per element. When the same element sits in different environments (NH₄NO₃, organic molecules, S₄O₆²⁻), the result is an average. Salts are also split into their ions where possible. For organic carbon atoms, draw the structure and assign each carbon from its bonds.

Working on redox mechanisms? Draw structures with formal charges and curved arrows in the free MolDraw editor.

[Open MolDraw editor](#)

Frequently asked questions

How do you know an oxidation number?

Apply the fixed rules (F -1, Group 1 +1, Group 2 +2, H +1, O -2, halogens -1) and solve for the remaining element so that the sum equals the overall charge.

How do you find the oxidation state of Cr in K₂Cr₂O₇?

K is +1 and O is -2: 2(+1) + 2x + 7(-2) = 0, so 2x = 12 and Cr = +6. In the ion Cr₂O₇²⁻ the answer is the same: 2x - 14 = -2.

How do I know if Fe is 2+ or 3+?

Use the charges of the other ions. FeCl₃ needs Fe³⁺ to balance three Cl⁻; FeO and FeSO₄ contain Fe²⁺. Fe₃O₄ contains both, so the average is +8/3.

Is Fe²⁺ to Fe³⁺ oxidation?

Yes. The oxidation number increases from +2 to +3 because iron loses one electron, and that is oxidation.

Why is the oxidation number of oxygen –1 in H₂O₂?

Hydrogen is +1, so two H contribute +2. The two oxygens must total –2, giving –1 each. The O–O bond does not change oxidation numbers.

Can oxidation numbers be fractions?

Yes, as averages. Fe₃O₄ gives +8/3 and S₄O₆^{2–} gives +2.5, because atoms of the same element are in different oxidation states.

Related chemistry tools

VSEPR molecular geometry calculator Shape, bond angles, hybridization in 3D
Chemical equation balancer Balance reactions and redox ions
Net ionic equation calculator Complete and net ionic equations
Electron configuration calculator Full and noble-gas notation
Lewis structure generator Lewis dot structures and VSEPR shape
Interactive periodic table All 118 elements with data
Molar mass calculator Step-by-step molar mass working
pH calculator pH, pOH, weak acids and buffers
Molecular weight calculator Formula to g/mol with % composition

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

PDB to PDBQT Converter Online | AutoDock PDBQT Tool

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

PDB to PDBQT converter online by MolDraw. Paste PDB text, upload a .pdb file, or import by PDB ID to generate a PDBQT draft with AutoDock atom type, charge, torsion, and format guidance.

In short: Paste PDB text, upload a .pdb file, or import by PDB ID to generate a PDBQT draft with AutoDock atom type, charge, torsion, and format guidance. It is free, works in your web browser and needs no download.

Paste a PDB structure, upload a .pdb file, or import a structure by PDB ID from the Protein Data Bank, then convert it into PDBQT for docking pipelines. This browser tool adds element and charge/type columns in PDBQT layout for fast preparation.

Quick answer: PDB stores structure coordinates, while PDBQT is a docking format that includes PDB-style coordinates plus partial charge and AutoDock atom type fields. Use this tool for a quick PDBQT draft from pasted text, a local PDB file, or an RCSB PDB ID before deeper ligand or receptor preparation.

PDB Input

Upload .pdb file

Paste PDB text, upload a local PDB file, or enter a 4-character PDB ID.

PDBQT Output

Ready.

Input and output formats

Input: PDB	Output: PDBQT	
Full name	PDB (Protein Data Bank format)	PDBQT (AutoDock format)
What it holds	3D atom coordinates in fixed columns. Used for proteins and small molecules.	PDB coordinates plus partial charges (Q) and AutoDock atom types (T), with torsion data for ligands.
File or form	.pdb	.pdbqt

Notes for Docking Workflows

- This tool creates a practical PDBQT text layout directly in-browser for rapid prototyping.
- For production docking runs, you can further refine protonation state and torsion definitions in your docking suite.
- Use this page as a quick conversion utility when you need a fast PDBQT draft structure.

How to convert PDB to PDBQT online

1. Paste PDB text, upload a local **.pdb** file, or type a 4-character PDB ID such as **1CRN**.
2. Click **Convert to PDBQT**. The converter keeps ATOM/HETATM coordinates and writes PDBQT-style charge and AutoDock atom type fields.
3. Copy or download the generated **.pdbqt** file for docking preparation, quick checks, or teaching examples.
4. Before a real docking run, review hydrogens, protonation, charges, atom types, flexible bonds, and receptor cleanup in your docking workflow.

PDB vs PDBQT

PDB is a general structural biology coordinate format. PDBQT is commonly used by AutoDock-style docking tools because it carries atom typing and partial charge information needed during docking calculations.

Format	What it stores	Common use
PDB	Atom names, residue names, chains, coordinates, occupancy, B-factor, and element symbols.	Protein structures, ligands, crystallography files, visualization, and structural biology exchange.

Format	What it stores	Common use
PDBQ	PDB-like coordinates plus partial charge information.	Older docking preparation workflows where charge is needed but AutoDock atom type is not stored as in PDBQT.
PDBQT	PDB-like coordinates plus partial charge and AutoDock atom type fields. Ligands may include torsion tree records.	AutoDock, AutoDock Vina, docking pipelines, ligand/receptor preparation, and docking tutorials.

Related docking and structure tools

[Protein Molecular Weight Calculator](#) [SMILES to PDBQT](#) [SMILES to PDB](#) [PDB to SMILES](#) [SMILES to 3D](#)

PDBQT Format Explained

A PDBQT file looks similar to a PDB file, but docking tools read extra fields near the end of each atom line. The **Q** part represents partial charge, and the **T** part represents the AutoDock atom type.

```
ATOM      1  N   ALA A   1       11.104  13.207   9.142  1.00 20.00   -0.346  N
ATOM      2  CA  ALA A   1       12.560  13.320   9.420  1.00 20.00    0.186  C
HETATM    3  O   LIG L   1       10.440  11.980   8.500  1.00 20.00   -0.508  OA
```

Atom types

AutoDock atom types such as **C**, **N**, **OA**, **SA**, **HD**, **Cl**, and **Zn** tell docking software how each atom should be interpreted during scoring.

Charges

PDBQT stores partial charges. This quick browser converter writes a neutral draft charge field, so production docking should still assign appropriate charges with a dedicated preparation tool.

Torsions

Flexible ligand PDBQT files can include **ROOT**, **BRANCH**, **ENDBRANCH**, and **TORSDOF** records to describe rotatable bonds and torsion degrees of freedom.

Receptors vs ligands

Receptor PDBQT preparation usually focuses on cleanup, hydrogens, charges, and atom types. Ligand PDBQT preparation also needs rotatable bond and torsion tree handling.

Important: MolDraw's browser output is a fast PDBQT draft. For AutoDock Vina production work, validate the protonation state, missing atoms, alternate locations, waters, metals, cofactors, charge model, atom typing, and ligand flexibility.

AutoDock Vina PDBQT Checklist

Use this checklist when preparing PDBQT files for AutoDock, AutoDock Vina, or related docking workflows.

- **Clean the PDB:** remove irrelevant waters, duplicated chains, alternate conformations, and non-target ligands unless they are needed.
- **Add hydrogens:** docking scores are sensitive to hydrogen placement, especially polar hydrogens and hydrogen-bond donors.
- **Check protonation:** choose the protonation state expected at your assay pH or biological condition.
- **Assign charges:** use a docking preparation workflow for realistic partial charges before final docking.
- **Review atom types:** metals, halogens, sulfur, phosphorus, and charged atoms may need careful atom typing.
- **Handle torsions:** ligand PDBQT files should define rotatable bonds correctly; receptor files are usually rigid unless flexible side chains are prepared separately.
- **Validate the output:** open the PDBQT in your docking or visualization tool before launching a long batch job.

PDBQT to PDB: what happens in reverse?

Searches such as **PDBQT to PDB converter** usually mean the user wants a simple coordinate file for viewing. A PDBQT file can often be reduced back to PDB-like ATOM/HETATM records by removing charge, atom type, and torsion tree metadata. However, PDB cannot preserve AutoDock-specific records such as ROOT, BRANCH, ENDBRANCH, and TORSDOF.

Common Questions

Is PDBQT the same as PDB?

No. PDB is a general coordinate format. PDBQT is a docking format that adds partial charge and AutoDock atom type fields, and may include torsion tree information for flexible ligands.

PDB to SMILES Converter

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

PDB to SMILES converter by MolDraw. Convert PDB structure text to SMILES using a best-effort public chemistry resolver workflow.

In short: Convert PDB structure text to SMILES using a best-effort public chemistry resolver workflow. It is free, works in your web browser and needs no download.

Paste PDB text and convert to SMILES with a best-effort resolver. For large proteins, use ligand-only PDB blocks.

SMILES output appears here.

Input and output formats

Input: PDB	Output: SMILES	
Full name	PDB (Protein Data Bank format)	SMILES (Simplified Molecular Input Line Entry System)
What it holds	3D atom coordinates in fixed columns. Used for proteins and small molecules.	Atoms, bonds, rings, charges and stereo as one line of text. No coordinates.
File or form	.pdb	.smi or plain text

File Format Explained

PDB stores 3D atom coordinates, residue names, chains, occupancy, B-factor, and element data. It is common for proteins, ligands, crystal structures, and molecular visualization.

SMILES stores a molecule as a compact line of connectivity text. It is best for small molecules and ligands, not full protein macromolecules.

For best results, convert ligand-only PDB blocks. Protein PDB files often contain many residues and missing bond-order information, so a direct PDB to SMILES conversion can be ambiguous.

Converting PDB ligands to SMILES

PDB files store atom coordinates, mainly for proteins and nucleic acids from crystallography, NMR, or cryo-EM. Small-molecule ligands appear as HETATM records. The format often lacks explicit bond orders for ligands, so converting coordinates into a SMILES string involves inferring bonds from atom distances and residue templates. That is why results are best-effort.

Getting good results

1. Extract only the ligand: copy its HETATM lines (and any CONECT lines for it) rather than the whole protein.
2. Remove water molecules (residue name HOH) and unrelated ions.
3. Convert and check the SMILES by drawing it with [SMILES to Structure](#).

Common issues

- **Missing hydrogens:** most crystal structures omit hydrogens, so bond orders and charges may need checking.
- **Wrong bond orders:** aromatic rings and carbonyls can be misassigned when geometry is distorted; compare with the ligand's entry in the PDB Chemical Component Dictionary.
- **Alternate conformations:** keep only one (for example altLoc A) to avoid duplicated atoms.

To view the protein itself, use the [Protein Viewer](#).

Related chemistry tools

[SMILES to PDB Converter](#)[CAS Number to SMILES Converter](#)[PDB to PDBQT Converter](#)
[OnlineCID to SMILES Converter](#)[InChI to SMILES Converter](#)[SMILES Notation Guide](#)

Percent Yield Calculator | Actual and Theoretical Yield

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

Percent yield calculator by MolDraw. Calculate percent yield, actual yield, or theoretical yield with gram, milligram, kilogram, mole, or mmol units.

In short: Calculate percent yield, actual yield, or theoretical yield with gram, milligram, kilogram, mole, or mmol units. It is free, works in your web browser and needs no download.

Calculate percent yield from actual and theoretical yield, or solve for actual/theoretical yield when percent yield is known.

Quick answer: percent yield = actual yield / theoretical yield × 100. Actual yield
Theoretical yield Percent yield (%) Result appears here.

Percent Yield Formula

- **Percent yield:** actual yield / theoretical yield × 100.
- **Actual yield:** theoretical yield × percent yield / 100.
- **Theoretical yield:** actual yield × 100 / percent yield.

[Molar Mass Calculator](#)[Empirical Formula Calculator](#)[Limiting reagent calculator](#)[Grams to moles calculator](#)[Molecular weight calculator](#)

Worked example

You react 5.00 g of salicylic acid (138.12 g/mol) with excess acetic anhydride to make aspirin (180.16 g/mol), and isolate 5.20 g of product.

1. Moles of salicylic acid = $5.00 \div 138.12 = 0.0362$ mol.
2. The reaction is 1:1, so the theoretical yield is $0.0362 \text{ mol} \times 180.16 \text{ g/mol} = 6.52$ g.
3. Percent yield = $5.20 \div 6.52 \times 100 = \mathbf{79.8\%}$.

Why yields fall below 100%

- Product lost during transfers, filtration, or recrystallisation.
- Incomplete reaction or competing side reactions.
- Equilibrium reactions that do not go fully to products.

Why a yield can appear above 100%

A result over 100% usually means the product is impure or wet: residual solvent, water, or unreacted starting material adds mass. Dry the product to constant mass and check purity,

for example by melting point or TLC.

Tip: theoretical yield must come from the limiting reagent. If you are unsure which reagent limits, convert every reagent to moles with the [Grams to Moles Calculator](#) and compare against the balanced equation.

Related chemistry tools

[Theoretical Yield Calculator](#)

pH Calculator - pH, pOH, Weak Acid & Buffer pH

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

Free pH calculator: find pH from [H+], strong or weak acid and base concentration, buffer pH (Henderson-Hasselbalch), pOH and pKa. Step-by-step.

In short: pH calculator: find pH from [H+], strong or weak acid and base concentration, buffer pH (Henderson-Hasselbalch), pOH and pKa. It is free, works in your web browser and needs no download.

Calculate pH, pOH, hydrogen ion concentration, hydroxide concentration, strong acid/base solution pH, dilution pH, buffer pH, and pKa values.

Quick answer: pH is $-\log_{10}[\text{H}^+]$. At 25 C, **pH + pOH = 14**. For buffers, use **pH = pKa + $\log_{10}(\text{base/acid})$** .

Presets

Choose a mode and enter values.

pH Calculator Formulas

pH from concentration

$$\text{pH} = -\log_{10}[\text{H}^+]$$

pOH relation

$$\text{pH} + \text{pOH} = 14 \text{ at } 25 \text{ C}$$

Hydrogen ion concentration

$$[\text{H}^+] = 10^{-\text{pH}}$$

Buffer pH

$$\text{pH} = \text{pKa} + \log_{10}(\text{base} / \text{acid})$$

When to Use Each pH Calculator Mode

- **pH level calculator:** use [H+] to pH or pH to [H+] modes.
- **pOH and pH calculator:** use pOH / [OH-] mode.

- **Solution pH calculator:** use strong acid/base mode for simple fully dissociated acids and bases.
- **Buffer pH calculator:** use Henderson-Hasselbalch mode for weak acid/conjugate base systems.
- **pH to pKa calculator:** use pKa from pH mode when base/acid ratio is known.

Assumptions: calculations use ideal behavior at 25 C unless stated otherwise. Pool pH adjustment, mixed acids/bases, ionic strength, activity coefficients, and real buffer capacity require more detailed chemistry than this educational calculator.

How to use the ph calculator

1. Pick a mode: *[H⁺] to pH, Strong acid/base, Weak acid/base, Buffer pH, Dilution or pKa from pH.*
2. Enter concentrations in mol/L. Scientific notation is accepted (1.8e-5).
3. Read pH, pOH and the ion concentration. Results update as you type.
4. Use the formula line under the result to show your working in a lab report.

Worked examples

0.010 M HCl (strong acid)

$$[\text{H}^+] = 0.010 \text{ M}$$

$$\text{pH} = -\log(0.010) = 2.00$$

0.10 M acetic acid, $K_a = 1.8 \times 10^{-5}$

$$x^2/(0.10 - x) = 1.8 \times 10^{-5} \rightarrow x = 1.33 \times 10^{-3} \text{ M}$$

$$\text{pH} = 2.88 \text{ (1.3\% ionised)}$$

0.10 M NH_3 , $K_b = 1.8 \times 10^{-5}$

$$[\text{OH}^-] = 1.33 \times 10^{-3} \text{ M}, \text{pOH} = 2.88$$

$$\text{pH} = 11.12$$

Acetate buffer, 0.10 M each

$$\text{pH} = 4.76 + \log(0.10/0.10)$$

$$\text{pH} = 4.76$$

Which pH formula should I use?

Situation	Formula
Known $[\text{H}^+]$	$\text{pH} = -\log[\text{H}^+]$
Strong acid, concentration C	$[\text{H}^+] = C \times (\text{H}^+ \text{ per formula}); \text{ e.g. } 0.05 \text{ M H}_2\text{SO}_4 \approx 0.10 \text{ M H}^+$

Situation	Formula
Strong base	$\text{pOH} = -\log[\text{OH}^-]$, $\text{pH} = 14 - \text{pOH}$
Weak acid (K_a)	$x^2/(C - x) = K_a$; if $x < 5\%$ of C , $x \approx \sqrt{K_a C}$
Buffer	$\text{pH} = \text{p}K_a + \log([A^-]/[HA])$ (Henderson-Hasselbalch)

All modes assume 25 °C ($K_w = 1.0 \times 10^{-14}$) and ideal dilute solutions. For very dilute strong acids and bases, the calculator includes water's own H^+/OH^- , so 10^{-8} M HCl correctly gives pH 6.98 rather than 8.

Preparing a buffer? Work out the masses with the solution prep calculator, then draw the acid-base structures in MolDraw.

[Solution prep calculator](#)

Frequently asked questions

How do you calculate pH?

$\text{pH} = -\log_{10}[\text{H}^+]$. For 0.01 M HCl, $[\text{H}^+] = 0.01$ M, so $\text{pH} = 2.00$. To go back, $[\text{H}^+] = 10^{-\text{pH}}$.

How do you calculate the pH of a weak acid?

Use K_a and the concentration: solve $x^2/(C - x) = K_a$ for $x = [\text{H}^+]$. For 0.10 M acetic acid ($K_a = 1.8 \times 10^{-5}$), $[\text{H}^+] = 1.33 \times 10^{-3}$ M and $\text{pH} = 2.88$.

What is the relationship between pH and pOH?

At 25 °C, $\text{pH} + \text{pOH} = 14$ because $K_w = [\text{H}^+][\text{OH}^-] = 1.0 \times 10^{-14}$.

How do you calculate the pH of a buffer?

Use the Henderson-Hasselbalch equation, $\text{pH} = \text{p}K_a + \log_{10}([A^-]/[HA])$. Equal acid and base concentrations give $\text{pH} = \text{p}K_a$.

Why is the pH of 10^{-8} M HCl not 8?

An acid cannot make water basic. At very low concentrations the H^+ from water (10^{-7} M) matters. Including it gives pH 6.98, which is what this calculator reports.

Does diluting an acid ten times raise the pH by one?

For a strong acid, yes, until the pH approaches 7. A tenfold dilution of pH 3 gives pH 4, but further dilution levels off at 7 rather than passing it.

Related chemistry tools

[Half-Life Calculator](#) Related tool [AP Chemistry Score Calculator](#) Related tool [Molarity calculator](#) Moles, volume and concentration [Dilution calculator](#) $C_1V_1 = C_2V_2$ dilutions [pKa calculator](#) Estimate acidity [Solution prep calculator](#) Mass needed for a solution [Net ionic](#)

equation calculator Complete and net ionic equations **Molar mass calculator** Step-by-step molar mass working **Grams to moles calculator** Convert mass and moles **Chemical equation balancer** Balance reactions and redox ions

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

pKa Calculator | pH to pKa and Henderson-Hasselbalch

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

pKa calculator by MolDraw. Calculate pKa from pH and base/acid ratio, pH from pKa, or Henderson-Hasselbalch buffer ratios.

In short: Calculate pKa from pH and base/acid ratio, pH from pKa, or Henderson-Hasselbalch buffer ratios. It is free, works in your web browser and needs no download.

Calculate pKa from pH and conjugate base/acid ratio, calculate buffer pH from pKa, or solve for the base/acid ratio with Henderson-Hasselbalch.

Quick answer: $\text{pH} = \text{pKa} + \log_{10}(\text{base} / \text{acid})$, so $\text{pKa} = \text{pH} - \log_{10}(\text{base} / \text{acid})$. Result appears here.

Henderson-Hasselbalch pKa Formula

- **pH:** $\text{pH} = \text{pKa} + \log_{10}(\text{base} / \text{acid})$.
- **pKa:** $\text{pKa} = \text{pH} - \log_{10}(\text{base} / \text{acid})$.
- **base/acid ratio:** $\text{base} / \text{acid} = 10^{(\text{pH} - \text{pKa})}$.

This educational calculator assumes ideal buffer behavior. Activity, ionic strength, temperature, and buffer capacity can shift real measured pH.

[pH calculator](#) [Molarity calculator](#) [Dilution calculator](#)

Using Henderson-Hasselbalch in practice

The equation $\text{pH} = \text{pKa} + \log_{10}([\text{A}^-]/[\text{HA}])$ links the pH of a buffer to the ratio of conjugate base to acid. When the two are equal, the log term is zero and $\text{pH} = \text{pKa}$. A buffer resists pH change best within about one pH unit of its pKa.

Worked example

An acetate buffer contains 0.10 M acetic acid and 0.15 M sodium acetate. Acetic acid has a pKa of about 4.76, so $\text{pH} = 4.76 + \log_{10}(0.15/0.10) = 4.76 + 0.18 = \mathbf{4.94}$.

Choosing a buffer

- Pick an acid whose pKa is close to the target pH: acetate (about 4.76) for pH 4–5.5, phosphate (pKa_2 about 7.2) near neutral pH.
- Higher total concentration gives more buffer capacity.

Limitations

The equation uses concentrations in place of activities, so it is an approximation. It becomes less reliable at high ionic strength, for very dilute buffers, and for strong acids or bases. pKa values also change with temperature. For accurate lab work, prepare the buffer and adjust with a calibrated pH meter.

Related chemistry tools

[Druglikeness Calculator](#)[Lipinski Rule Calculator](#)[TPSA Calculator](#)[LogP Calculator](#)[SMILES to Molecular Weight Calculator](#)[Mass Spectrum Predictor](#)

Protein Molecular Weight Calculator - kDa & ϵ_{280}

<https://www.moldraw.com/tools/free-chem-tools/protein-molecular-weight-calculator.html>

Calculate protein or peptide molecular weight from its sequence: average and monoisotopic mass in Da/kDa, composition and extinction coefficient at 280 nm.

In short: Calculate protein or peptide molecular weight from its sequence: average and monoisotopic mass in Da/kDa, composition and extinction coefficient at 280 nm. It is free, works in your web browser and needs no download.

Paste a protein or peptide sequence (one-letter codes or FASTA). You get the average and monoisotopic molecular weight, amino-acid composition, and the molar extinction coefficient and A_{280} of a 1 mg/mL solution for UV concentration measurements.

Quick answer: protein MW = sum of residue masses + one water (18.015 Da). The insulin A chain (21 residues) is **2383.71 Da** average, 2382.00 Da monoisotopic. Protein / peptide sequence (FASTA headers, spaces and numbers are ignored) Results appear here.

How to use the protein molecular weight calculator

1. Paste the sequence in one-letter code. FASTA format is fine because the header line, spaces, numbers and line breaks are removed.
2. The calculator adds the average (or monoisotopic) residue mass of every amino acid, plus one water for the free N- and C-termini.
3. Read the molecular weight in Da and kDa. Use average mass for SDS-PAGE and buffers, and monoisotopic mass for high-resolution mass spectrometry of peptides.
4. Use the extinction coefficient with Beer-Lambert ($c = A_{280} / \epsilon \cdot l$) to find concentration from a UV reading.

Worked examples

Insulin A chain (21 aa)

GIVEQCCTSICSLYQLENYCN

2383.71 Da average · 2382.00 Da monoisotopic

$$\epsilon_{280} = 2 \text{ Tyr} \times 1490 + 2 \text{ cystines} \times 125 = 3230 \text{ M}^{-1}\text{cm}^{-1}$$

Human ubiquitin (76 aa)

8564.84 Da (8.56 kDa)

One Tyr, no Trp: $\epsilon_{280} = 1490 \text{ M}^{-1}\text{cm}^{-1}$

Concentration from A_{280}

A protein with $\epsilon = 43,824 \text{ M}^{-1}\text{cm}^{-1}$ reads $A_{280} = 0.55$ in a 1 cm cuvette.

$$c = 0.55 \div 43,824 = 12.6 \text{ } \mu\text{M}$$

How protein molecular weight is calculated

When amino acids join, each peptide bond releases one water, so a protein is a chain of *residues* (amino acid minus H_2O) plus one water for the terminal H and OH:

$$\text{MW} = \sum (\text{residue mass}) + 18.015 \text{ Da (average)} \quad \text{MW}_{\text{mono}} = \sum (\text{monoisotopic residue mass}) + 18.011 \text{ Da}$$

Average residue masses use natural isotope abundances and are what SDS-PAGE, gel filtration and weighing relate to. Monoisotopic masses use only the most abundant isotope (^{12}C , ^1H , ^{14}N , ^{16}O , ^{32}S) and match the first peak in a high-resolution mass spectrum of a peptide. A quick estimate is 110 Da per residue.

Extinction coefficient at 280 nm

Absorbance at 280 nm comes from Trp, Tyr and disulfide-bonded cysteines. Using the Pace et al. (1995) values:

$\epsilon_{280} = 5500 \times n(\text{Trp}) + 1490 \times n(\text{Tyr}) + 125 \times n(\text{cystine})$ The calculated mass is for the unmodified polypeptide chain. Glycosylation, phosphorylation, disulfide bonds (–2.016 Da each), signal-peptide removal and N-terminal Met processing all change the real mass. Ambiguous codes (B, Z, X) are not accepted; U (selenocysteine) and O (pyrrolysine) are.

For small molecules use the [molecular weight calculator](#); to view a protein structure from the PDB, open the [MolDraw protein viewer](#).

Studying a protein-ligand complex? View PDB structures in 3D and prepare ligands for docking with MolDraw's free tools.

[Open protein viewer](#)

Frequently asked questions

How do you calculate the molecular weight of a protein?

Add the residue mass of every amino acid in the sequence and add 18.015 Da for one water. The average residue mass is about 110 Da, so 300 residues is roughly 33 kDa.

What is the difference between average and monoisotopic mass?

Average mass uses natural isotope abundances and suits bulk measurements. Monoisotopic mass uses only the lightest stable isotopes and matches high-resolution mass spectrometry of peptides.

How do I convert Da to kDa?

Divide by 1000. 8564.84 Da = 8.56 kDa. One dalton equals 1 g/mol.

How is the extinction coefficient calculated?

$\epsilon_{280} = 5500 \times \text{Trp} + 1490 \times \text{Tyr} + 125 \times \text{cystines (M-1 cm-1)}$. Two values are given, depending on whether the cysteines form disulfides.

Why does my protein run at a different size on SDS-PAGE?

Post-translational modifications, unusual charge or incomplete unfolding change gel mobility. The calculated value is for the unmodified chain.

Does the calculator handle FASTA format?

Yes. Header lines that start with '>' are ignored, as are spaces, line breaks, numbers and stop symbols (*).

Related chemistry tools

Protein Viewer pluginPDB in 3D
Molecular weight calculatorFormula to g/mol with % composition
Exact mass calculatorMonoisotopic mass for MS
Molarity calculatorMoles, volume and concentration
Dilution calculator $C1V1 = C2V2$ dilutions
PDB to PDBQT converterPrepare files for docking
Molar mass calculatorStep-by-step molar mass working
Solution prep calculatorMass needed for a solution
SMILES to molecular weightMW straight from a SMILES string

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

SDF to InChI Converter

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

SDF to InChI converter by MolDraw. Convert SDF or MOL blocks into standard InChI strings for indexing and search.

In short: Convert SDF or MOL blocks into standard InChI strings for indexing and search. It is free, works in your web browser and needs no download.

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

InChI output appears here.

Input and output formats

Input: SDF	Output: InChI	
Full name	SDF (Structure Data File)	InChI (IUPAC International Chemical Identifier)
What it holds	One or more MOL records, each with optional data fields, split by \$\$\$\$.	A layered text identifier built from the structure. The standard InChI is the same in every program.
File or form	.sdf	Text starting with InChI=1S/

File Format Explained

SDF stores molecule records with MOL-style atom and bond blocks plus optional property fields. It is common for compound libraries and screening datasets.

InChI is a standardized IUPAC identifier that represents a molecule in layered text form. Converting SDF to InChI helps create stable identifiers for search, indexing, and deduplication.

If an SDF contains multiple records, convert and verify records carefully. Structure salts, mixtures, stereochemistry, and missing hydrogens can affect the resulting InChI.

About SDF files

An SDF (structure-data file) is essentially many MOL records joined together. Each record is followed by optional data fields such as > <NAME> or > <CAS> and ends with a line containing \$\$\$\$.

Compound libraries, PubChem downloads, and supplier catalogues commonly use SDF because one file can hold thousands of molecules with their properties.

Why generate InChI

Standard InChI gives every structure a canonical identifier, independent of atom order and drawing. That is useful for merging libraries, removing duplicates, and matching compounds against public databases.

How to use it

1. Open the .sdf file in a plain-text editor.
2. Copy a record (from its header through \$\$\$\$) and paste it in.
3. Convert and copy the InChI, or shorten it with [InChI to InChIKey](#).

Troubleshooting

- Records with unusual elements, query atoms, or R-groups may not produce a standard InChI.
- Large files are easier to handle a few records at a time.

- Keep the original spacing; SDF connection tables are column-based.

Related chemistry tools

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

SDF to InChIKey Converter

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

SDF to InChIKey converter by MolDraw. Convert SDF or MOL blocks to standard InChIKey identifiers for database matching.

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

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

InChIKey output appears here.

Input and output formats

Input: SDF	Output: InChIKey	
Full name	SDF (Structure Data File)	InChIKey
What it holds	One or more MOL records, each with optional data fields, split by \$\$\$\$.	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	.sdf	Text like XXXXXXXXXXXXXXX-YYYYYYYYY-Z

File Format Explained

SDF is a structure-data format that can store atom/bond blocks and compound properties. It is widely used for chemical datasets and screening libraries.

InChIKey is a compact hashed identifier derived from an InChI. It is especially useful for database matching, indexing, and checking whether two records likely describe the same compound.

InChIKey is search-friendly but not fully reversible. Keep the source SDF if you need coordinates, atom blocks, or property fields later.

Using InChIKeys with compound libraries

When you receive a compound library as SDF, an InChIKey for each record gives you a short, searchable fingerprint of the structure. Keys fit neatly in spreadsheets and databases and make it easy to spot the same compound listed under different names or IDs.

How to use it

1. Copy one or more SDF records, each ending with \$\$\$\$.
2. Paste and convert.
3. Copy the resulting 27-character keys into your spreadsheet next to the compound IDs.

Practical uses

- **Deduplication:** sort by InChIKey; identical keys indicate the same structure, including stereochemistry.
- **Finding stereoisomers:** group by the first 14-character block to collect compounds that share a skeleton but differ in stereo or isotopes.
- **Cross-referencing:** search keys in public databases to find literature, suppliers, or safety data.

Note: salts and mixtures in SDF records produce keys for the whole record, so a hydrochloride salt and its free base have different keys. Strip counter-ions first if you want to match parent compounds. For the full identifier, use [SDF to InChI](#).

Related chemistry tools

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

What Is SMILES? SMILES Notation Guide, Rules & Codes (with Validator)

<https://www.moldraw.com/tools/free-chem-tools/smiles-notation-guide.html>

Learn SMILES notation: what SMILES is, the rules for atoms, bonds, branches, rings, aromaticity and stereo, SMILES codes for common molecules, and a live SMILES validator with 2D preview.

In short: Learn SMILES notation: what SMILES is, the rules for atoms, bonds, branches, rings, aromaticity and stereo, SMILES codes for common molecules, and a live SMILES validator with 2D preview. It is free, works in your web browser and needs no download.

SMILES writes a molecule as a line of text. This guide covers every rule you need, with worked examples and a table of SMILES codes for common molecules. A live validator checks your SMILES, gives its formula and draws it.

Quick answer: SMILES lists atoms as symbols (hydrogens are implicit), uses = and # for double and triple bonds, () for branches, matching digits for rings and lower case for aromatic atoms. Ethanol is CCO and benzene is c1ccccc1. Try a SMILES string ([live validator](#))

What is SMILES?

SMILES (Simplified Molecular Input Line Entry System) is a way of writing a chemical structure as a single line of ASCII text. David Weininger introduced it in 1988 (*J. Chem. Inf.*

Comput. Sci. 28, 31–36). Today the OpenSMILES specification documents it. A SMILES string lists atoms in the order you would meet them walking through the molecule, with symbols for bonds, branches and ring closures. Ethanol is CCO, benzene is c1ccccc1 and caffeine is Cn1cnc2c1c(=O)n(C)c(=O)n2C.

Because it is plain text, SMILES is the standard way to store, search and exchange molecules in databases (PubChem, ChEMBL), spreadsheets, code and machine-learning datasets. It can be typed or copied into almost any chemistry program, including MolDraw.

SMILES rules in 8 steps

Rule	How it works	Examples
Atoms	Organic-subset atoms B, C, N, O, P, S, F, Cl, Br, I are written as bare symbols. Hydrogens are added automatically to fill normal valence.	C methane, O water, N ammonia, CCl chloromethane
Brackets	Any other element, charge, isotope or explicit H goes in square brackets, and then no hydrogens are added automatically.	[Na+], [NH4+], [O-], [13CH4], [Fe+2]
Bonds	Single bonds are implied between neighbours. Write = for double, # for triple, and . to separate pieces that are not bonded.	CC ethane, C=C ethene, C#N HCN, [Na+] . [Cl-]
Branches	A branch goes in parentheses after the atom it is attached to. Branches can be nested.	CC(C)C isobutane, CC(=O)O acetic acid
Rings	Break one bond of the ring and label both ends with the same digit. Digits can be reused once a ring is closed, and %10 and up are used for very large ring counts.	C1CCCCC1 cyclohexane, C1CC1 cyclopropane
Aromaticity	Lower-case atoms are aromatic, and the bonds between them are aromatic. Kekulé form with alternating = bonds is also valid.	c1ccccc1 = C1=CC=CC=C1 benzene; c1cc[nH]c1 pyrrole
Stereo (cis/trans)	/ and \ show the direction of bonds on each side of a double bond.	F/C=C/F trans, F/C=C\F cis-1,2-difluoroethene
Stereo (chirality)	@ (anticlockwise) or @@ (clockwise) inside brackets give the order of neighbours seen from the first one.	C[C@@H](C(=O)O)N L-alanine

Writing a SMILES by hand: isobutanol

1. Draw the skeleton without hydrogens: $(\text{CH}_3)_2\text{CH}-\text{CH}_2-\text{OH}$.
2. Pick a starting atom at one end, e.g. a methyl carbon: C.
3. Walk to its neighbour, the CH carbon: CC. It has a second methyl, written as a branch: CC(C).
4. Continue along the main chain to the CH_2 and then the O: CC(C)CO.
5. Hydrogens are implicit, so CC(C)CO is complete: $\text{C}_4\text{H}_{10}\text{O}$.

Many SMILES can describe the same molecule (OCC(C)C is also isobutanol). A **canonical SMILES** is the single standard version a program produces, so identical molecules give identical strings. An **isomeric SMILES** also keeps stereochemistry and isotopes.

SMILES codes of common molecules

SMILES from PubChem, with formulas checked by this page's parser. Tap *Try* to load one into the validator.

Molecule	SMILES	Formula
Acetic acid	<chem>CC(=O)O</chem>	C ₂ H ₄ O ₂
Acetone	<chem>CC(=O)C</chem>	C ₃ H ₆ O
Adrenaline (epinephrine)	<chem>CNC[C@@H](C1=CC(=C(C=C1)O)O)O</chem>	C ₉ H ₁₃ NO ₃
Ammonia	<chem>N</chem>	H ₃ N
Aspirin	<chem>CC(=O)OC1=CC=CC=C1C(=O)O</chem>	C ₉ H ₈ O ₄
Benzene	<chem>C1=CC=CC=C1</chem>	C ₆ H ₆
Caffeine	<chem>CN1C=NC2=C1C(=O)N(C(=O)N2C)C</chem>	C ₈ H ₁₀ N ₄ O ₂
Carbon dioxide	<chem>C(=O)=O</chem>	CO ₂
Cholesterol	<chem>C[C@H](CCCC(C)C)[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CC=C4[C@@]3(CC[C@@H](C4)O)C)C</chem>	C ₂₇ H ₄₆ O
Citric acid	<chem>C(C(=O)O)C(CC(=O)O)(C(=O)O)O</chem>	C ₆ H ₈ O ₇
Cyclohexane	<chem>C1CCCCC1</chem>	C ₆ H ₁₂
Ethanol	<chem>CCO</chem>	C ₂ H ₆ O
Ethene	<chem>C=C</chem>	C ₂ H ₄
Ethyne	<chem>C#C</chem>	C ₂ H ₂
Glucose	<chem>C([C@@H]1[C@H]([C@@H]([C@H](C(O1)O)O)O)O)O</chem>	C ₆ H ₁₂ O ₆
Glycine	<chem>C(C(=O)O)N</chem>	C ₂ H ₅ NO ₂
Ibuprofen	<chem>CC(C)Cc1ccc(cc1)C(C)C(=O)O</chem>	C ₁₃ H ₁₈ O ₂
L-Alanine	<chem>C[C@@H](C(=O)O)N</chem>	C ₃ H ₇ NO ₂
Methane	<chem>C</chem>	CH ₄
Methanol	<chem>CO</chem>	CH ₄ O
Naphthalene	<chem>c1ccc2ccccc2c1</chem>	C ₁₀ H ₈
Paracetamol	<chem>CC(=O)Nc1ccc(O)cc1</chem>	C ₈ H ₉ NO ₂
Phenol	<chem>Oc1ccccc1</chem>	C ₆ H ₆ O
Pyridine	<chem>c1ccncc1</chem>	C ₅ H ₅ N
Serotonin	<chem>C1=CC2=C(C=C1)C(=CN2)CCN</chem>	C ₁₀ H ₁₂ N ₂ O

Molecule	SMILES	Formula
Sodium chloride	<chem>[Na+].[Cl-]</chem>	ClNa
Sucrose	<chem>C([C@@H]1[C@H]([C@@H]([C@H]([C@H](O1)O[C@]2([C@H]([C@@H]([C@H](O2)CO)O)O)CO)O)O)O</chem>	C ₁₂ H ₂₂ O ₁₁
Toluene	<chem>Cc1ccccc1</chem>	C ₇ H ₈
Vanillin	<chem>COc1cc(C=CC(=C1)C=O)O</chem>	C ₈ H ₈ O ₃
Water	<chem>O</chem>	H ₂ O

Common SMILES mistakes

- **Unclosed rings:** C1CC opens ring 1 but never closes it.
- **Valence errors:** C(C)(C)(C)(C)C gives carbon five bonds.
- **Aromatic N-H:** pyrrole is c1cc[nH]c1, and the bracketed [nH] is required.
- **Case matters:** Co is cobalt, while CO is methanol, and Sc is scandium, not S plus aromatic C.
- **Charges need brackets:** write [O-], not O-.

Convert SMILES to other formats

MolDraw has free converters for every common direction: [SMILES to structure \(2D\)](#), [structure to SMILES](#), [name to SMILES](#), [SMILES to IUPAC name](#), [SMILES to InChI](#), [SMILES to MOL](#) and [SMILES to 3D](#).

SMILES to 3D Structure Converter - View & Download

<https://www.moldraw.com/tools/free-chem-tools/smiles-to-3d-structure-converter.html>

Convert SMILES to an interactive 3D structure in your browser. Rotate, style and download SDF, PDB, XYZ, MOL or PNG. Free SMILES to 3D converter.

In short: Convert SMILES to an interactive 3D structure. It is free, works in your web browser and needs no download.

SMILES Input

3D Structure Output

Ready.

Input and output formats

Input: SMILES	Output: 3D structure	
Full name	SMILES (Simplified Molecular Input Line Entry System)	3D structure

Input: SMILES	Output: 3D structure	
What it holds	Atoms, bonds, rings, charges and stereo as one line of text. No coordinates.	A model with x, y, z coordinates for every atom, shown as a rotatable view.
File or form	.smi or plain text	On screen, with file downloads

File Format Explained

SMILES is a compact text representation of molecular connectivity. It is excellent for input, search, and database workflows, but it does not directly store a final 3D conformation.

3D structure formats such as SDF, XYZ, PDB, MOL, OBJ, and X3D store coordinates or renderable geometry. SDF and PDB are chemistry coordinate formats, XYZ is a simple atom-coordinate table, and OBJ/X3D are 3D model formats for visualization workflows. Use the [XYZ / Gaussian to 2D converter](#) when you need to turn coordinate files back into an inferred 2D drawing. To predict the VSEPR shape, bond angles and hybridization around a central atom, try the [VSEPR molecular geometry calculator](#).

Generated 3D coordinates are useful for visualization and teaching. For docking, quantum chemistry, or publication-quality geometry, validate protonation, stereochemistry, conformer quality, and force-field optimization.

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

Related chemistry tools

[SMILES to InChI Converter](#)[SMILES to InChIKey Converter](#)[SMILES to IUPAC Name Converter](#)[SMILES to MOL Converter](#)[SMILES Notation Guide](#)[SMILES to Structure Converter](#)
[Online 3D Molecular Model Viewer](#)

SMILES to InChI Converter

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

SMILES to InChI converter by MolDraw. Convert SMILES strings to standard InChI identifiers for database and publication workflows.

In short: Convert SMILES strings to standard InChI identifiers for database and publication workflows. It is free, works in your web browser and needs no download.

Convert SMILES to standard InChI for search, indexing, and publication workflows.

InChI output appears here.

Input and output formats

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

File Format Explained

SMILES is a compact line notation for molecular connectivity. It is convenient for drawing tools, search boxes, and scripts.

InChI is the IUPAC International Chemical Identifier. It is a layered, standardized identifier designed for chemical database exchange, indexing, and comparison.

Use SMILES when you need an editable structure string. Use InChI when you need a standardized identifier that is less dependent on a specific SMILES canonicalization style.

Example and reading the output

Aspirin's SMILES CC(=O)OC1=CC=CC=C1C(=O)O converts to:

InChI=1S/C9H8O4/c1-6(10)13-8-5-3-2-4-7(8)9(11)12/h2-5H,1H3,(H,11,12)

- 1S: version 1, standard InChI.
- C9H8O4: the molecular formula layer.
- /c...: the connectivity layer, using InChI's own atom numbering.
- /h...: where the hydrogens sit; the brackets mark a mobile hydrogen shared between the two carboxylic acid oxygens.

Why the same molecule always gives the same InChI

Several different SMILES can describe aspirin, depending on which atom you start from. Standard InChI is canonical, so all of them produce the identical string above. This makes InChI a good choice for comparing structures and checking duplicates.

FAQ

Is stereochemistry included? Yes. @ and @@ in SMILES become /t, /m and /s layers in the InChI. **Need something shorter?** Use [SMILES to InChIKey](#).

Related chemistry tools

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

SMILES to InChIKey Converter

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

SMILES to InChIKey converter by MolDraw. Convert SMILES strings into searchable InChIKey identifiers.

In short: Convert SMILES strings into searchable InChIKey identifiers. It is free, works in your web browser and needs no download.

Generate compact InChIKey identifiers from SMILES strings.

InChIKey output appears here.

Input and output formats

Input: SMILES	Output: InChIKey	
Full name	SMILES (Simplified Molecular Input Line Entry System)	InChIKey
What it holds	Atoms, bonds, rings, charges and stereo as one line of text. No coordinates.	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	.smi or plain text	Text like XXXXXXXXXXXXXXX-YYYYYYYYYY-Z

File Format Explained

SMILES is a compact text notation for molecular structure. It is useful for input, editing, and conversion workflows.

InChIKey is a fixed-length hashed identifier derived from an InChI. It is designed for fast database matching and web search, but it cannot be reversed perfectly without a database lookup.

Use InChIKey when you need a stable search key for a compound; use SMILES when you need an editable structure string.

Why use an InChIKey

InChIKeys are designed for searching. Pasting a full InChI or SMILES into a search engine often fails, because symbols such as =, /, and parentheses are treated specially. A 27-character key made only of letters and hyphens searches cleanly and matches database records reliably.

Example

Caffeine, CN1C=NC2=C1C(=O)N(C(=O)N2C)C, gives the InChIKey RYYVLZVUVIJVGH-UHFFFA0YSA-N. Searching that key returns pages for caffeine in PubChem, ChEMBL, and other databases.

Structure of the key

- **First 14 characters:** hash of the connectivity.
- **Next 10 characters:** hash of stereochemistry and isotope layers, plus version flags. UHFFFA0YSA appears for structures with no stereo or isotope layers.
- **Last character:** protonation (N = neutral).

FAQ

Do enantiomers get different keys? Yes, if the stereochemistry is defined in the SMILES. They share the first block and differ in the second. **Can I get the structure back from a key?** Only by database lookup, using [InChIKey to SMILES](#).

Related chemistry tools

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

SMILES to IUPAC Name Converter - Free & Instant

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

Convert SMILES to an IUPAC name instantly, including stereo (E/Z, R/S). Paste SMILES or import from PubChem by name or CID. Free, no sign-up.

In short: Convert SMILES to an IUPAC name instantly, including stereo (E/Z, R/S). It is free, works in your web browser and needs no download.

Convert SMILES to IUPAC names for reports, assignments, naming checks, and chemical identifier workflows.

Quick answer: Paste a SMILES string, import a compound from PubChem, or try an example. MolDraw returns the matching IUPAC name from PubChem when a matching compound record is available.

Tip: complex research codes such as calderasib or FMC-376 may resolve only if PubChem has a matching record.

IUPAC name output appears here.

Input and output formats

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

Input: SMILES	Output: IUPAC name	
File or form	.smi or plain text	Text

File Format Explained

SMILES is a compact molecular line notation used for search, conversion, and cheminformatics workflows. It is optimized for machines rather than formal naming.

IUPAC names are systematic chemical names intended to describe compounds in formal language. They are useful in reports, assignments, publications, and naming checks.

One molecule may have multiple acceptable names or equivalent SMILES strings. Database-backed naming works best for recognized compounds with clear connectivity, charge, and stereochemistry.

How this SMILES to IUPAC converter works

The tool sends the SMILES string to PubChem's property lookup and displays the returned IUPAC name. You can also search PubChem first by compound name or CID, import the PubChem SMILES, and convert it automatically.

- Use SMILES for compact molecule identifiers.
- Use IUPAC names for formal reports, naming checks, and searchable chemical descriptions.
- If no result is found, verify stereochemistry, charges, salts, and unusual fragments in the SMILES input.
- For uncommon drug codes or research compounds, try both the code name and PubChem CID if available.

Related chemistry tools

[SMILES to structure](#)[SMILES to InChI](#)[SMILES to InChIKey](#)[IUPAC to SMILES](#)[Draw structure → IUPAC name](#)

Don't have the SMILES? Draw the molecule and get its IUPAC name directly.

[Structure to IUPAC name](#)

Frequently asked questions

How do I convert SMILES to an IUPAC name?

Paste the SMILES string and click Convert. MolDraw sends it to PubChem, which standardises the structure and returns its computed IUPAC name, including stereodescriptors.

Why does a SMILES with / or \ fail on other converters?

Slashes (E/Z double bonds) and # (triple bonds) break URL-based lookups. This converter sends SMILES in the request body, so stereo SMILES such as C/C=C/C(=O)O work and return

(E)-but-2-enoic acid.

Can it name a molecule that is not in PubChem?

Usually not. Automatic naming relies on PubChem's database of over 100 million compounds. For new structures, name them by hand or name a close analogue and adapt it.

Can I draw a structure instead of typing SMILES?

Yes. Use the Structure to IUPAC Name tool, which has a built-in editor: draw the molecule and the name updates automatically.

Is the SMILES to IUPAC converter free?

Yes. It is free with no sign-up and runs in your browser.

Which name does it return for drugs like aspirin?

The systematic IUPAC name, e.g. 2-acetyloxybenzoic acid for aspirin, not the trade or common name.

Need to sketch the structure? [Draw chemical structures online](#) with MolDraw, a free [online ChemDraw alternative](#).

Related chemistry tools

[SMILES Notation Guide](#)

SMILES to MOL Converter

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

SMILES to MOL converter by MolDraw. Convert SMILES strings into MOL structure files for compatibility workflows.

In short: Convert SMILES strings into MOL structure files for compatibility workflows. It is free, works in your web browser and needs no download.

Convert SMILES to downloadable MOL format for editor and ELN compatibility.

MOL output appears here.

Input and output formats

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

Input: SMILES	Output: MOL file	
File or form	.smi or plain text	.mol

File Format Explained

SMILES is a compact one-line text identifier for a molecule. It is easy to paste into databases, scripts, and web tools, but it does not store a drawn 2D layout.

MOL, also called a molfile, stores atom and bond tables with coordinates. Use MOL when an editor, ELN, or cheminformatics tool needs an editable structure file instead of a text identifier.

After conversion, check stereochemistry, charges, and aromatic rings before using the MOL file in publication, registration, or computational workflows.

What a MOL file contains

SMILES describes which atoms are bonded, but it carries no coordinates. A MOL file adds a 2D layout: each atom gets x and y coordinates, so other programs can display the molecule without recalculating a layout. That makes MOL a safe choice when you move a structure into ChemDraw-compatible software, electronic lab notebooks, or registration systems.

Reading the output

- **Lines 1-3:** header (name, program, comment).
- **Counts line:** number of atoms and bonds, plus the version tag V2000.
- **Atom block:** one line per atom with x, y, z coordinates and element symbol.
- **Bond block:** pairs of atom numbers and the bond type (1 single, 2 double, 3 triple).
- M END closes the record.

How to use it

1. Paste a SMILES such as CCO (ethanol).
2. Convert and download or copy the MOL text.
3. Save it with a .mol extension and open it in your target program.

Need several molecules in one file? Use [SMILES to SDF](#). Need 3D coordinates for modelling? Try [SMILES to PDB](#).

Related chemistry tools

[MOL to SMILES Converter](#)[SMILES to 3D Structure Converter](#)[SMILES to InChI Converter](#)[SMILES to InChIKey Converter](#)[SMILES Notation Guide](#)[SMILES to Structure Converter Online](#)

SMILES to MOL2 Converter

<https://www.moldraw.com/tools/free-chem-tools/smiles-to-mol2-converter.html>

SMILES to MOL2 converter by MolDraw. Convert SMILES strings into MOL2 format for docking and med-chem workflows.

In short: Convert SMILES strings into MOL2 format for docking and med-chem workflows. It is free, works in your web browser and needs no download.

Convert SMILES strings to MOL2 format for docking and pipeline compatibility.

MOL2 output appears here.

Input and output formats

Input: SMILES	Output: MOL2	
Full name	SMILES (Simplified Molecular Input Line Entry System)	MOL2 (Tripos Mol2)
What it holds	Atoms, bonds, rings, charges and stereo as one line of text. No coordinates.	3D coordinates, bonds, atom types and partial charges.
File or form	.smi or plain text	.mol2

File Format Explained

SMILES stores molecule connectivity in a short line of text. It is useful for identifiers, but it does not carry Tripos atom typing or molecule sections.

MOL2 is the Tripos Mol2 format. It can store atoms, bonds, substructures, atom types, coordinates, and charges, which makes it useful in docking, molecular modeling, and medicinal chemistry workflows.

Use MOL2 when a docking or modeling tool expects Tripos atom types or charge fields. Validate protonation, charges, and generated coordinates before production docking.

When you need MOL2

MOL2 is a common input format for docking, virtual screening, and molecular mechanics. Besides coordinates, it stores SYBYL atom types and partial charges, which many modelling programs rely on. Converting a SMILES string to MOL2 is a quick way to prepare a ligand when you only have its structure as text.

How to use it

1. Paste the SMILES of your ligand, for example ibuprofen
CC(C)CC1=CC=C(C=C1)C(C)C(=O)O.
2. Convert and download the .mol2 file.
3. Open it in your modelling or docking software.

Before docking

- **Protonation:** decide what charge state is relevant at your target pH. A carboxylic acid such as ibuprofen is mostly deprotonated at pH 7.4.
- **Stereochemistry:** specify @ or @@ in the SMILES for chiral centres; otherwise the generated geometry may pick one arbitrarily.
- **Geometry:** generated 3D coordinates are a starting conformer; energy minimisation in your modelling package is usually recommended.

For docking programs that need PDBQT, see [SMILES to PDBQT](#). To go back, use [MOL2 to SMILES](#).

Related chemistry tools

[SMILES to 3D Structure Converter](#)[SMILES to InChI Converter](#)[SMILES to InChIKey Converter](#)[SMILES Notation Guide](#)[SMILES to Structure Converter Online](#)[Structure to SMILES Converter](#)

SMILES to Molecular Formula Converter

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

SMILES to molecular formula converter by MolDraw. Paste a SMILES string and get molecular formula, molecular weight, IUPAC name, and PubChem CID when available.

In short: Paste a SMILES string and get molecular formula, molecular weight, IUPAC name, and PubChem CID when available. It is free, works in your web browser and needs no download.

Paste a SMILES string to get the molecular formula and supporting PubChem metadata.

Quick answer: paste SMILES such as **CCO** or **CC(=O)OC1=CC=CC=C1C(=O)O**, then convert to formula. Molecular formula output appears here.

About SMILES and Molecular Formula

SMILES describes molecular connectivity as a compact text string. A molecular formula summarizes the atom counts in the molecule, such as C₉H₈O₄ for aspirin.

- Use formula output for reports, exact mass checks, and composition calculations.
- Use the molecular weight tool when you need g/mol from the formula.

[Molar Mass Calculator](#)[Empirical Formula Calculator](#)[SMILES to molecular weight](#)[Exact mass calculator](#)[Molecular weight calculator](#)

How the formula is worked out

SMILES lists heavy atoms explicitly, but most hydrogens are implicit: each atom gets enough hydrogens to fill its normal valence. To build the formula, the tool counts every explicit atom, adds the implicit hydrogens, and writes the result in Hill order: carbon first, hydrogen second, then all other elements alphabetically.

Worked example

For ethyl acetate, CCOC(=O)C:

- Carbons: 4. Oxygens: 2.
- Hydrogens: CH3 (3) + CH2 (2) + the ester carbon (0) + CH3 (3) = 8.
- Formula: **C₄H₈O₂**.

Things to watch

- **Charges:** CC(=O)[O-] (acetate) gives C2H3O2-, one hydrogen fewer than acetic acid.
- **Bracket atoms:** atoms in square brackets get only the hydrogens written, so [CH2] is a carbon with exactly two.
- **Salts:** dotted SMILES such as [Na+].[Cl-] combine all components.

Need mass too? Use [SMILES to Molecular Weight](#) or the [Exact Mass Calculator](#).

Related chemistry tools

[Degree of Unsaturation Calculator](#)

SMILES to Molecular Weight Calculator

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

SMILES to molecular weight converter by MolDraw. Paste a SMILES string and get molecular weight, formula, IUPAC name, and PubChem CID when available.

In short: Paste a SMILES string and get molecular weight, formula, IUPAC name, and PubChem CID when available. It is free, works in your web browser and needs no download.

Paste a SMILES string to calculate molecular weight and retrieve the matching formula when PubChem has a compound record.

Quick answer: paste SMILES and calculate molecular weight in g/mol. Molecular weight output appears here.

How SMILES Molecular Weight Lookup Works

The tool resolves the SMILES string through PubChem and reads the molecular weight property from the matched compound record.

- For formula-only workflows, use the molecular weight calculator.
- For mass spectrometry formula checks, use exact mass instead of average molecular weight.

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

Molecular weight versus exact mass

Molecular weight (molar mass) is calculated from standard atomic weights, which average over natural isotope abundances: about 12.011 for carbon, 1.008 for hydrogen, 15.999 for oxygen, and 14.007 for nitrogen. It is the value to use for weighing reagents and preparing solutions. Exact (monoisotopic) mass uses only the most abundant isotope of each element and is the value to compare with high-resolution mass spectra.

Worked example

Aspirin, CC(=O)OC1=CC=CC=C1C(=O)O, is $C_9H_8O_4$.

$9 \times 12.011 + 8 \times 1.008 + 4 \times 15.999 = 108.099 + 8.064 + 63.996 = \mathbf{180.16 \text{ g/mol}}$. Its monoisotopic mass is about 180.042 Da.

Practical uses

- To make 100 mL of a 0.1 M solution, you need 0.01 mol, which is 1.80 g of aspirin.
- For hydrates and salts, include the counter-ion and water in the SMILES so the weight matches the bottle you are weighing from.

Continue with the [Grams to Moles](#) or [Solution Prep](#) calculators.

SMILES to NMR | Predict ^1H and ^{13}C NMR from SMILES

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

Predict ^1H and ^{13}C NMR from SMILES. Paste a structure string, choose a nucleus, and see predicted chemical shifts and a spectrum. This is a prediction, not an experimental NMR spectrum.

In short: Paste a structure string, choose a nucleus, and see predicted chemical shifts and a spectrum. It is free, works in your web browser and needs no download.

Paste a SMILES string and predict ^1H and ^{13}C NMR chemical shifts. The result is a predicted shift table and spectrum, not an experimental measurement.

Quick answer: paste SMILES, pick ^1H or ^{13}C , and predict NMR shifts. This is a prediction, not an experimental spectrum. Nucleus ^1H ^{13}C Sign in to predict NMR spectra.

Shift (ppm)	Integral	Multiplicity	Coupling (Hz)
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Predicted chemical shifts only. This is not an experimental NMR spectrum.

How SMILES to NMR works

The tool sends your SMILES string to the NMR prediction service already used by the MolDraw NMR analyser. ^1H predictions use the proton endpoint and ^{13}C predictions use the carbon endpoint. Shifts are grouped the same way as that plugin and drawn as a predicted spectrum.

- Use a single organic molecule SMILES string.
- Switch between ¹H and ¹³C after the first prediction to run the other nucleus.
- Treat the table as a guide. Solvent and experimental conditions are not part of this prediction.

[NMR viewer \(open your spectrum\)](#) [Structure to NMR](#) [Structure to SMILES](#) [SMILES to structure](#)
[Mass spectrum predictor](#)

FAQ

Is SMILES to NMR an experimental spectrum?

No. SMILES to NMR predicts ¹H or ¹³C chemical shifts from the SMILES you paste. The table and plot are a model prediction, not a measured NMR spectrum.

How do I predict ¹H and ¹³C NMR from SMILES?

Paste a SMILES string, choose ¹H or ¹³C, and click Predict NMR. The page sends that SMILES to the same NMR prediction service the MolDraw NMR analyser uses and lists the predicted shifts.

Why can predicted shifts differ from a textbook spectrum?

The service predicts shifts for the structure you entered. It does not include solvent, temperature, concentration, or impurities. Compare the table with an experimental spectrum before you publish assignments.

Related chemistry tools

[How to read an NMR spectrum](#)[NMR Analyser plugin \(1H, 13C, 2D\)](#)[SMILES to 3D Structure Converter](#)[SMILES to InChI Converter](#)[SMILES to InChIKey Converter](#)[SMILES to IUPAC Name Converter](#)[SMILES Notation Guide](#)[IUPAC Name to SMILES Converter](#)[Degree of Unsaturation Calculator](#)[IR Spectroscopy Chart \(Correlation Table\)](#)

SMILES to PDB Converter

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

SMILES to PDB converter by MolDraw. Convert a SMILES string to a downloadable 3D PDB file with a free chemistry tool.

In short: Convert a SMILES string to a downloadable 3D PDB file. It is free, works in your web browser and needs no download.

Convert a SMILES string to a 3D PDB file using a public chemistry conversion endpoint. You can preview and download the generated PDB text.

PDB output appears here.

Input and output formats

Input: SMILES	Output: PDB	
Full name	SMILES (Simplified Molecular Input Line Entry System)	PDB (Protein Data Bank format)
What it holds	Atoms, bonds, rings, charges and stereo as one line of text. No coordinates.	3D atom coordinates in fixed columns. Used for proteins and small molecules.
File or form	.smi or plain text	.pdb

File Format Explained

SMILES is a compact text identifier for molecular connectivity. It is easy to paste and store, but it does not contain explicit 3D coordinates.

PDB stores atom coordinates in a structural biology format. PDB is useful for 3D visualization, molecular modeling, and workflows that expect coordinate files.

A SMILES to PDB conversion generates a coordinate draft from connectivity. Validate stereochemistry, protonation, and conformer geometry before using the PDB in docking or computational chemistry.

What you get and how to use it

The converter generates a 3D conformer from the SMILES connectivity and writes it as PDB, with one HETATM line per atom giving its x, y, z coordinates in ångströms. This is useful for viewing a small molecule in 3D software, preparing a ligand for modelling, or creating a quick 3D picture for teaching.

How to use it

1. Paste a SMILES, for example caffeine CN1C=NC2=C1C(=O)N(C(=O)N2C)C.
2. Convert and preview the PDB text.
3. Download the .pdb file and open it in a molecular viewer.

Things to know

- **One conformer:** flexible molecules have many shapes. The file contains one reasonable geometry, not necessarily the bioactive or lowest-energy one.
- **Stereochemistry:** specify @/@@ for chiral centres and / or \ for double-bond geometry, otherwise the geometry may be chosen arbitrarily.
- **Bond orders:** the PDB format does not reliably store bond orders, so some programs re-infer them. If you need bond orders preserved, consider [SMILES to MOL2](#) or [SMILES to SDF](#).

For docking with AutoDock-family tools, use [SMILES to PDBQT](#).

Related chemistry tools

[PDB to SMILES Converter](#)[SMILES to 3D Structure Converter](#)[PDB to PDBQT Converter](#)
[Online SMILES to InChI Converter](#)[SMILES to InChIKey Converter](#)[SMILES Notation Guide](#)

SMILES to PDBQT Converter

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

SMILES to PDBQT converter by MolDraw. Convert a SMILES string into PDBQT format for molecular docking and AutoDock-style workflows.

In short: Convert a SMILES string into PDBQT format for molecular docking and AutoDock-style workflows. It is free, works in your web browser and needs no download.

Convert SMILES to PDBQT in two steps: generate a 3D PDB from SMILES, then transform the structure into PDBQT text for docking-ready workflows.

Ready.

Input and output formats

Input: SMILES	Output: PDBQT	
Full name	SMILES (Simplified Molecular Input Line Entry System)	PDBQT (AutoDock format)
What it holds	Atoms, bonds, rings, charges and stereo as one line of text. No coordinates.	PDB coordinates plus partial charges (Q) and AutoDock atom types (T), with torsion data for ligands.
File or form	.smi or plain text	.pdbqt

Technical Workflow

- Step 1: the tool requests 3D PDB coordinates from a public SMILES conversion endpoint.
- Step 2: PDB atom lines are rewritten into PDBQT-style records with atom type and charge columns.
- Use this quick converter for drafts; fine-tune protonation and torsion settings in docking software when needed.

File Format Explained

SMILES is a compact connectivity string. It is good for describing a ligand quickly, but it does not contain docking atom types, charges, torsions, or 3D coordinates.

PDBQT is an AutoDock-style docking format. It stores PDB-like coordinates plus partial charge and AutoDock atom type fields, and ligand files may include torsion tree records such as ROOT, BRANCH, ENDBRANCH, and TORSDOF.

This converter creates a browser-side PDBQT draft. For production AutoDock Vina docking, review hydrogens, protonation, charge model, atom typing, and rotatable bonds.

Related chemistry tools

[PDB to PDBQT Converter](#) [Online](#) [SMILES to 3D Structure Converter](#) [SMILES to InChI Converter](#) [SMILES to InChIKey Converter](#) [SMILES Notation Guide](#) [SMILES to Structure Converter](#) [Online](#)

SMILES to SDF Converter

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

SMILES to SDF converter by MolDraw. Convert SMILES strings into SDF format for screening and dataset workflows.

In short: Convert SMILES strings into SDF format for screening and dataset workflows. It is free, works in your web browser and needs no download.

Convert SMILES to SDF for dataset and virtual screening pipelines.

SDF output appears here.

Input and output formats

Input: SMILES	Output: SDF	
Full name	SMILES (Simplified Molecular Input Line Entry System)	SDF (Structure Data File)
What it holds	Atoms, bonds, rings, charges and stereo as one line of text. No coordinates.	One or more MOL records, each with optional data fields, split by \$\$\$\$.
File or form	.smi or plain text	.sdf

File Format Explained

SMILES is a compact string representation of molecular connectivity. It is convenient for search and exchange, but it usually does not include rich metadata.

SDF is a structure-data file format that can store one or many molecule records, usually with MOL-style atom/bond blocks plus optional property fields. SDF is common in screening libraries, compound datasets, and cheminformatics pipelines.

Use SDF when you need a file that can carry structure records and compound properties together. Review stereochemistry and generated coordinates before batch use.

Why SDF

SDF (structure-data file) stores one or more structures, each as a MOL connection table followed by optional named data fields and a \$\$\$\$ separator. It is the standard way to move

compound sets between cheminformatics tools, compound registration systems, and databases, because properties such as IDs, names, or assay results can travel with each structure.

How to use it

1. Paste a SMILES, for example paracetamol CC(=O)NC1=CC=C(C=C1)O.
2. Convert and download the .sdf file.
3. Open it in your chemistry software, or combine several converted files into one library.

Example record layout

- Header lines, then the counts line with atom and bond numbers.
- The atom block (coordinates and elements) and the bond block.
- M END, then any data fields such as > <NAME> followed by a value.
- \$\$\$\$ to close the record.

FAQ

How is SDF different from MOL? A MOL file holds one structure; an SDF can hold many, with data. **Can I go back to identifiers?** Yes, with [SDF to InChIKey](#) or [SDF to InChI](#).

Related chemistry tools

[SMILES to 3D Structure Converter](#)[SMILES to InChI Converter](#)[SMILES to InChIKey Converter](#)[SMILES to IUPAC Name Converter](#)[SMILES Notation Guide](#)[SMILES to Structure Converter Online](#)

SMILES to Structure Converter Online | Draw 2D Molecules

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

SMILES to structure converter online by MolDraw. Paste SMILES or import a compound from PubChem, render a 2D chemical structure, and download SVG, PNG, or JPG.

In short: Paste SMILES or import a compound from PubChem, render a 2D chemical structure, and download SVG, PNG, or JPG. It is free, works in your web browser and needs no download.

Paste a SMILES string and render a compact 2D chemical structure instantly. Download the molecule drawing as SVG, PNG, or JPG.

Quick answer: This free online tool converts SMILES to a 2D structure drawing in the browser and lets you export the rendered molecule as SVG, PNG, or JPG.

SMILES Input

Structure Output

Copy Ready.

Convert SMILES to a chemical structure image

SMILES is compact and machine-readable, but reports, slides, and teaching materials often need a visible 2D structure. This converter draws the molecule from the SMILES string and provides image downloads for quick reuse.

File Format Explained

SMILES is a one-line molecular notation that stores connectivity in text form. It is ideal for databases and converters, but not for human-friendly visual layout.

SVG is a vector image format, best for crisp structures in slides and documents. **PNG** and **JPG** are raster image formats, useful for quick sharing, web uploads, and reports.

- Use SVG for crisp vector graphics in documents and presentations.
- Use PNG for transparent raster images in web or slide workflows.
- Use JPG when a white-background image is preferred.

Related SMILES tools

[Structure to IUPAC Name](#) [SMILES to IUPAC](#) [SMILES to InChI](#) [SMILES to 3D](#) [SMILES to MOL file](#) [SMILES to SDF](#) [SMILES to molecular weight](#) [InChIKey to SMILES](#) [Open MolDraw editor](#)

Related guides

[Free chemical databases to find SMILES](#) [All free MolDraw chemistry tools](#) [MolDraw video tutorials](#) [Free MolDraw course](#)

Related chemistry tools

[VSEPR Molecular Geometry Calculator](#) & [ChartSMILES Notation Guide](#)

Solution Prep Calculator

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

Solution prep calculator by MolDraw. Calculate required solute mass for target molarity and final solution volume.

In short: Calculate required solute mass for target molarity and final solution volume. It is free, works in your web browser and needs no download.

Calculate required solute mass from target molarity, molecular weight, and final solution volume.

Target molarity (M) Final volume (mL) Molecular weight (g/mol) Enter valid values.

How much solute to weigh

To make a solution of a target molarity, weigh **mass (g) = molarity (mol/L) × final volume (L) × molecular weight (g/mol)**. Example: 250 mL of 0.1 M NaCl (58.44 g/mol) needs $0.1 \times 0.250 \times 58.44 = 1.461$ g.

Dissolve the solute in less solvent than you need, then make it up to the final volume in a volumetric flask. If your reagent is a hydrate, use the molecular weight of the hydrate form.

Working in millimolar: divide by 1000 first, so 50 mM is 0.050 M. **Example:** 500 mL of 50 mM glucose (180.16 g/mol) needs $0.050 \times 0.500 \times 180.16 = 4.50$ g. Use an analytical balance for small masses, and record the exact mass weighed so you can calculate the true concentration afterwards.

Stoichiometry Calculator - Grams, Moles, Particles & Gas Volume

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

Free stoichiometry calculator: type any reaction, give an amount of one species in grams, moles, particles, gas litres or solution volume, and get the amount of any other species with step-by-step mole-ratio working.

In short: Stoichiometry calculator: type any reaction, give an amount of one species in grams, moles, particles, gas litres or solution volume, and get the amount of any other species with step-by-step mole-ratio working. It is free, works in your web browser and needs no download.

Convert between any two substances in a reaction. Type the equation (it is balanced for you), enter what you know in grams, moles, particles, litres of gas or a solution volume, and get the answer in the unit you need. A full table shows every reactant and product, with each step explained.

Quick answer: grams A $\div$ M(A) $\rightarrow$ mol A $\times$ (b/a) $\rightarrow$ mol B $\times$ M(B) $\rightarrow$ grams B. Burning **10.0 g propane** ($\text{C}_3\text{H}_8 + 5\text{O}_2 \rightarrow 3\text{CO}_2 + 4\text{H}_2\text{O}$) needs **36.3 g O₂**. Chemical equation (balanced automatically) Given species Amount Given unit Molarity (M) Find species Answer unit Gas conditions T (°C) P (atm)

How to solve stoichiometry problems

1. **Balance the equation.** The coefficients give the mole ratio.
2. **Convert what you are given to moles:** grams $\div$ molar mass, particles $\div 6.022 \times 10^{23}$, litres of gas $\div 22.4$ L/mol (STP), or volume of solution $\times$ molarity.
3. **Apply the mole ratio:** mol B = mol A $\times$ (coefficient of B $\div$ coefficient of A).
4. **Convert moles of B** into the unit you need (grams, particles, litres).

grams A $\rightarrow \div$ M(A) $\rightarrow$ mol A $\rightarrow \times$ (b/a) $\rightarrow$ mol B $\rightarrow \times$ M(B) $\rightarrow$ grams B

Convert	To moles	From moles
Mass (g)	$\div$ molar mass	$\times$ molar mass
Particles	$\div 6.022 \times 10^{23}$	$\times 6.022 \times 10^{23}$
Gas volume (L)	$\div 22.414$ L/mol (STP)	$\times 22.414$ L/mol
Solution volume (L)	$\times$ molarity	$\div$ molarity

Worked examples

Mass to mass

How much O₂ burns 10.0 g propane? $\text{C}_3\text{H}_8 + 5\text{O}_2 \rightarrow 3\text{CO}_2 + 4\text{H}_2\text{O}$. $10.0/44.10 = 0.2268 \text{ mol} \times 5 = 1.134 \text{ mol} \times 32.00$

36.3 g O₂

Moles to gas volume

1 mol Fe₂O₃ + 3CO → 2Fe + 3CO₂ gives 3 mol CO₂ × 22.414 L/mol

67.2 L CO₂ at STP

Solution stoichiometry

25.0 mL of 0.200 M H₂SO₄ = 5.00 mmol, which needs 2 × 5.00 = 10.0 mmol NaOH × 40.00 g/mol

0.400 g NaOH

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 stoichiometry?

Stoichiometry uses the mole ratios in a balanced chemical equation to work out how much of one substance reacts with, or forms from, a given amount of another.

How do you do grams-to-grams stoichiometry?

Convert grams of A to moles (÷ molar mass), multiply by the mole ratio (coefficient of B ÷ coefficient of A), then convert moles of B to grams (× molar mass of B).

What is the mole ratio?

The ratio of coefficients in the balanced equation. In $2\text{H}_2 + \text{O}_2 \rightarrow 2\text{H}_2\text{O}$ the mole ratio of H₂ to O₂ is 2:1, so 4 mol H₂ needs 2 mol O₂.

What molar volume should I use for gases?

22.414 L/mol at STP (0 °C, 1 atm), 22.711 L/mol at IUPAC STP (0 °C, 1 bar) and 24.465 L/mol at 25 °C and 1 atm. For other conditions use $V = nRT/P$, which the custom option does.

How do I handle solutions?

Moles = molarity × volume in litres. For example, 25.0 mL of 0.200 M = 0.00500 mol. Then apply the mole ratio as usual.

What if one reactant runs out?

This calculator converts between two species, assuming everything else is in excess. If you have amounts of two or more reactants, use the theoretical yield calculator to find the limiting reagent.

Related chemistry tools

Theoretical yield calculator Limiting reagent → grams of product
Chemical equation balancer Balance any reaction
Grams to moles calculator Mass ↔ moles
Ideal gas law calculator $PV = nRT$
Molarity calculator Solution concentration
Limiting reagent calculator Find the limiting reactant

Structure to IUPAC Name - Draw & Get Name Free

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

Draw a chemical structure and get its IUPAC name instantly. Free IUPAC name generator with a built-in molecule editor, SMILES input and PubChem lookup.

In short: Draw a chemical structure and get its IUPAC name instantly. It is free, works in your web browser and needs no download.

Draw a molecule in the editor (or paste SMILES) and get its systematic IUPAC name, molecular formula and PubChem record. Stereochemistry you draw (wedges, E/Z) is included in the name.

Quick answer: draw the structure, then click *Get IUPAC name*. For example, the structure of aspirin returns **2-acetyloxybenzoic acid**.

Loading editor...

SMILES (filled from the drawing, or paste your own) Draw a structure or paste SMILES, then click Get IUPAC name. [Open in MolDraw editor](#)

How to use the structure to iupac name

1. Draw the molecule in the editor using the bond and atom tools, or type a SMILES string into the box.
2. The SMILES updates as you draw, and after a short pause the name is looked up automatically. You can also click *Get IUPAC name*.
3. Read the IUPAC name, molecular formula and molecular weight. Follow the PubChem link for properties, synonyms and safety data.
4. Click *Open in MolDraw editor* to keep working on the structure, add it to a reaction scheme or export an image.

Worked examples

Aspirin

CC(=O)Oc1ccccc1C(=O)O

2-acetyloxybenzoic acid

(E)-crotonic acid

C/C=C/C(=O)O

(E)-but-2-enoic acid

The E descriptor comes from the double-bond geometry you draw.

Ibuprofen

CC(C)Cc1ccc(cc1)C(C)C(=O)O

2-[4-(2-methylpropyl)phenyl]propanoic acid

How the IUPAC name is generated

The editor converts your drawing to a SMILES string. That string is sent to PubChem, which standardises the structure and returns the IUPAC name it has computed for that compound (PubChem holds over 100 million compounds). Stereochemistry in the drawing is preserved. If the exact stereoisomer is not in PubChem, the tool retries without stereo and tells you, so you can add R/S or E/Z yourself.

Limitation: automatic naming works for compounds that exist in PubChem. Brand-new structures from your own synthesis may return no name; then use the rules below, or name a close analogue and adapt it.

Naming an organic compound by hand (short version)

1. **Find the principal functional group** (carboxylic acid > ester > amide > nitrile > aldehyde > ketone > alcohol > amine). It sets the suffix: -oic acid, -al, -one, -ol...
2. **Choose the parent chain or ring** that contains that group and is longest: meth-, eth-, prop-, but-, pent-, hex-...
3. **Number the chain** so the principal group, then multiple bonds, then substituents get the lowest locants.
4. **Name substituents** in alphabetical order with locants (2-methyl, 4-chloro), using di-, tri- for repeats.
5. **Add stereodescriptors** (R/S, E/Z) in front.

Already have a SMILES string? Use the [SMILES to IUPAC name converter](#). For the reverse direction use [IUPAC name to SMILES](#).

Need publication-quality structures? MolDraw is a free online ChemDraw alternative with templates, reactions and image export.

[Open full MolDraw editor](#)

Frequently asked questions

How do I get the IUPAC name from a structure?

Draw the structure in the editor on this page or paste its SMILES. The tool looks up the systematic IUPAC name from PubChem and shows it with the formula and molecular weight.

Is this IUPAC name generator free?

Yes. It runs in your browser with the free MolDraw editor and public PubChem data. No sign-up is needed.

Does it include stereochemistry?

Yes. Wedge bonds and double-bond geometry are encoded in the SMILES and returned as R/S and E/Z in the name when PubChem has that stereoisomer.

Why do I get 'No IUPAC name found'?

PubChem can only name structures in its database. Check for drawing errors such as wrong valences or missing charges. A genuinely new compound has to be named by hand.

Can I get a name from a picture of a structure?

Not directly. Redraw the structure in the editor (it takes seconds for most molecules) or convert the image to SMILES first.

What is the difference between an IUPAC name and a common name?

An IUPAC name is systematic and describes the structure (2-acetyloxybenzoic acid). A common or trade name such as aspirin is shorter but carries no structural information.

Related chemistry tools

Build a Molecule Related tool **SMILES to IUPAC name** Convert SMILES to a systematic name **IUPAC name to SMILES** Name to SMILES and structure **Structure to SMILES** Draw and copy SMILES **SMILES to structure** Draw a structure from SMILES **Molecular weight calculator** Formula to g/mol with % composition **Lewis structure generator** Lewis dot structures and VSEPR shape **Chemical reaction drawer** Draw reaction schemes online **Exact mass calculator** Monoisotopic mass for MS

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

Structure to NMR | Predict ¹H and ¹³C NMR from a Drawn Structure

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

Structure to NMR lets you draw a molecule and predict ¹H and ¹³C NMR chemical shifts. Predict NMR reads SMILES from the embedded editor. The spectrum is a prediction, not an

experimental result.

In short: Structure to NMR lets you draw a molecule and predict ^1H and ^{13}C NMR chemical shifts. It is free, works in your web browser and needs no download.

Draw a molecule on the left and predict ^1H and ^{13}C NMR on the right. Predict NMR reads the SMILES from the editor, then shows predicted shifts. This is not an experimental spectrum.

Quick answer: draw a structure, choose ^1H or ^{13}C , and click Predict NMR to predict shifts from that structure. 2D editor Loading editor

How Structure to NMR reads the editor

This page embeds the MolDraw editor at `/embed?bridge=1`, the same embed used by Structure to SMILES. Predict NMR sends a get-smiles message to that frame and predicts from the SMILES string the editor returns.

- Draw or load an example, then click Predict NMR.
- The right-hand SMILES box shows the string that was predicted.
- The shift table and plot are predicted values, not a laboratory spectrum.

[NMR viewer \(open your spectrum\)](#) [SMILES to NMR](#) [Structure to SMILES](#) [SMILES to structure](#) [Mass spectrum predictor](#)

FAQ

How does Structure to NMR read the drawing?

The left pane embeds the same MolDraw 2D editor used by other structure tools. Predict NMR asks that frame for the current SMILES, then predicts ^1H or ^{13}C shifts from that string.

Is the Structure to NMR spectrum experimental?

No. The plot and shift table are predicted ^1H or ^{13}C NMR values. They are not an experimental spectrum.

What if Predict NMR does not return shifts?

Wait until the editor says it is ready, draw one organic molecule, then click Predict NMR. An empty canvas or a structure the model cannot parse will not produce a shift table.

Related chemistry tools

[How to read an NMR spectrum](#)[NMR Analyser plugin \(1H, 13C, 2D\)](#)[Structure to IUPAC Name Generator](#)[SMILES Notation Guide](#)[IUPAC Name to SMILES Converter](#)[IR Spectroscopy Chart \(Correlation Table\)](#)[Degree of Unsaturation Calculator](#)[Molecular Formula Finder](#)

Structure to SMILES Converter | Draw Molecule and Get SMILES

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

Structure to SMILES converter by MolDraw. Draw a molecule in the 2D editor and get the SMILES string in realtime.

In short: Draw a molecule in the 2D editor and get the SMILES string in realtime. It is free, works in your web browser and needs no download.

Draw or edit a molecule in the 2D editor on the left. The SMILES string updates on the right as the structure changes.

Quick answer: draw a molecule in the editor and copy the realtime SMILES output.

2D Structure Editor

Loading editor...

How Structure to SMILES Works

This page embeds the existing MolDraw 2D editor and listens for realtime editor messages. When the MolDraw editor updates the molecule, the tool reads the generated SMILES and displays it in the output box.

- Use it when you want to sketch a molecule and immediately copy a SMILES string.
- Check stereochemistry, charges, aromaticity, and salts before using SMILES in databases or modeling workflows.
- For the reverse workflow, use the SMILES to Structure tool.

[Structure to IUPAC Name](#) [SMILES to structure](#) [SMILES to IUPAC](#) [SMILES to formula](#) [SMILES to 3D](#)

Related chemistry tools

[SMILES Notation Guide](#)

Theoretical Yield Calculator - Limiting Reagent & Percent Yield

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

Free theoretical yield calculator: type any reaction, enter reactant masses or moles, and get the balanced equation, limiting reagent, theoretical yield in grams, leftover excess and percent yield, step by step.

In short: Theoretical yield calculator: type any reaction, enter reactant masses or moles, and get the balanced equation, limiting reagent, theoretical yield in grams, leftover excess and percent yield, step by step. It is free, works in your web browser and needs no download.

Enter a chemical equation and the amounts of your reactants. The calculator balances the equation, finds the limiting reagent and works out the theoretical yield of any product in grams and moles. Add your actual yield to get the percent yield.

Quick answer: convert reactants to moles, divide each by its coefficient to find the **limiting reagent**, multiply by the product/reactant mole ratio, then by the product's molar mass. 2.00 g salicylic acid gives a theoretical yield of **2.61 g aspirin**. Chemical equation (balanced automatically) ProductActual yield (g, optional)

How to calculate theoretical yield

1. **Balance the equation.** The calculator does this for you using its [equation balancer](#).
2. **Convert each reactant to moles:** mass $\div$ molar mass.
3. **Find the limiting reagent:** divide each reactant's moles by its coefficient. The smallest value is limiting.
4. **Use the mole ratio:** mol product = mol limiting $\times$ (product coefficient $\div$ limiting coefficient).
5. **Convert to grams:** theoretical yield = mol product $\times$ molar mass of product.

Theoretical yield (g) = (mol limiting reagent) $\times$ (b/a) $\times$ M(product) Percent yield = actual $\div$ theoretical $\times$ 100%

Worked examples

Aspirin from salicylic acid

2.00 g $C_7H_6O_3$ (0.01448 mol) with 5.00 g acetic anhydride (0.04898 mol), 1:1 ratio. Salicylic acid is limiting: 0.01448×180.16 g/mol

Theoretical yield 2.609 g. If 1.80 g is isolated, the yield is 69.0%

Haber process

28.0 g N_2 (0.9995 mol) + 10.0 g H_2 (4.96 mol). $N_2 + 3H_2 \rightarrow 2NH_3$, so N_2 is limiting: 1.999 mol $NH_3 \times 17.03$ g/mol

34.04 g NH_3

Water synthesis

10 g H_2 (4.96 mol) + 64 g O_2 (2.00 mol). $2H_2 + O_2 \rightarrow 2H_2O$, so O_2 is limiting: 4.00 mol H_2O

72.06 g H_2O ; 1.94 g H_2 left over

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 theoretical yield?

Theoretical yield is the maximum amount of product that could form if the limiting reagent reacted completely, with no losses. You calculate it from the balanced equation and the molar masses.

How do you find the limiting reagent?

Convert each reactant to moles and divide by its coefficient in the balanced equation. The reactant with the smallest result runs out first. That is the limiting reagent, and it sets the theoretical yield.

What is the difference between theoretical, actual and percent yield?

Theoretical yield is calculated, actual yield is what you isolate in the lab, and percent yield = $\text{actual} \div \text{theoretical} \times 100\%$.

Can percent yield be over 100%?

Not for a pure, dry product. A result above 100% usually means the product still contains solvent or water, or is contaminated, or there was a weighing error.

What if I only know the amount of one reactant?

Enter just that reactant and leave the others blank. They are treated as being in excess, so the reactant you entered is limiting.

Do I need to balance the equation first?

No. Type the unbalanced equation (e.g. $\text{C}_3\text{H}_8 + \text{O}_2 \rightarrow \text{CO}_2 + \text{H}_2\text{O}$) and the calculator balances it before working out the mole ratios.

Related chemistry tools

Stoichiometry calculator Grams, moles and gas volumes
Limiting reagent calculator Find the limiting reactant
Percent yield calculator Actual vs theoretical yield
Chemical equation balancer Balance any reaction
Molar mass calculator g/mol from a formula
Ideal gas law calculator $PV = nRT$
Grams to moles calculator Mass $\leftrightarrow$ moles

TLC Diagram Tool Online | Thin Layer Chromatography Plate Maker

<https://www.moldraw.com/tools/free-chem-tools/tlc-diagram-tool.html>

Free TLC diagram maker for thin layer chromatography. Draw TLC plates with lanes, spots, solvent front, baseline, Rf labels, and export SVG or PNG for lab reports.

In short: TLC diagram maker for thin layer chromatography. It is free, works in your web browser and needs no download.

Create a thin layer chromatography plate diagram directly on this page. Add lanes, edit Rf spots, show solvent front and baseline labels, then export the plate as SVG or PNG.

Title Solvent system Stationary phase Plate width Plate height Solvent front height (% of run) 18% Show Rf labels

Quick TLC Workflow

Quick answer: A TLC plate diagram should show the baseline, solvent front, sample lanes, compound spots, lane labels, solvent system, stationary phase, and Rf values when they are known.

- Define plate size and solvent front clearly.
- Add lanes and label samples consistently.
- Record spot distances and compute Rf values.
- Export final plate visualization for notebook and report use.

TLC Diagram Maker for Lab Reports

This thin layer chromatography diagram maker is designed for common searches such as **TLC plate drawing**, **chromatography plate diagram**, **Rf value diagram**, and **TLC lab report figure**. It helps students, teachers, and lab teams create a clean visual plate without redrawing the same baseline, solvent front, and spots by hand.

What to include in a TLC plate diagram

Show the origin line or baseline near the bottom, a dashed solvent front near the top, separate sample lanes, visible spots, lane labels, and the solvent system used for the run.

When to show Rf labels

Rf labels are useful for lab reports, teaching slides, and compound comparison. Hide them when you only need a clean qualitative plate illustration.

How to Calculate Rf Value

In thin layer chromatography, the Rf value compares how far a compound spot moved with how far the solvent front moved from the baseline. The value is unitless and usually falls between 0 and 1.

$$R_f = \text{distance travelled by compound spot} / \text{distance travelled by solvent front}$$

For example, if a spot moves 3.2 cm and the solvent front moves 5.0 cm, the Rf value is 0.64. In this diagram tool you can enter that value directly for each spot, and the plate preview places the spot proportionally between the baseline and solvent front.

Common TLC Diagram Uses

Organic chemistry labs

Use TLC diagrams to compare reactant, product, co-spot, and crude reaction mixture lanes during reaction monitoring.

Teaching and worksheets

Create simple TLC plates for explaining polarity, solvent choice, spot separation, UV visualization, staining, and Rf interpretation.

Purification reports

Illustrate column fractions, purification checks, and before/after comparisons using labeled lanes and colored spots.

Notebook figures

Export SVG for editable vector diagrams or PNG for quick insertion into electronic lab notebooks and reports.

Related chemistry tools

[Draw a chemical reaction in your browser](#)[Chemical Equation Balancer](#)[Structure to SMILES Converter](#)[Build a Molecule](#)[Lewis Structure Generator](#)[Name to Structure Tool](#)

TPSA Calculator | Topological Polar Surface Area

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

Free TPSA calculator for SMILES or compound names. Retrieve topological polar surface area, molecular formula, molecular weight, IUPAC name, and CID.

In short: TPSA 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 topological polar surface area (TPSA), a common medicinal chemistry property for permeability and oral bioavailability screening.

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

What TPSA Tells You

TPSA estimates the polar surface contributed by hetero atoms and attached hydrogens. In Veber-style oral bioavailability guidelines, TPSA at or below about 140 Å² is often considered favorable, although context matters.

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

Interpreting TPSA

Topological polar surface area (TPSA) adds up surface contributions from polar atoms, mainly oxygen and nitrogen and the hydrogens attached to them. Ertl and colleagues introduced the fragment-based method in 2000 so the value can be computed from the 2D structure alone, without generating a 3D model. That makes it fast enough to screen large libraries.

Commonly used thresholds

- **140 Å² or less:** part of Veber's criteria associated with good oral bioavailability in rats.
- **About 90 Å² or less:** often cited for compounds intended to cross the blood-brain barrier.

Examples

- Aspirin: about 63.6 Å² (an ester and a carboxylic acid).
- Ibuprofen: about 37.3 Å² (one carboxylic acid).
- Glucose: about 110 Å² (five hydroxyl groups and a ring oxygen).

Keep in mind: TPSA ignores sulfur and phosphorus in its standard form, and it is a guide, not a measurement of permeability. Use it together with logP and molecular weight, for example in the [Druglikeness Calculator](#).

Related chemistry tools

[Compare molecules](#) [pluginKa Calculator](#) [SMILES to Molecular Weight Calculator](#) [Mass Spectrum Predictor](#)

VSEPR Chart & Molecular Geometry Calculator (3D)

<https://www.moldraw.com/tools/free-chem-tools/vsepr-molecular-geometry-calculator.html>

Free VSEPR calculator and molecular geometry chart: enter a formula, name or SMILES to get AXE class, electron and molecular geometry, bond angles, hybridization and polarity in 3D.

In short: VSEPR calculator and molecular geometry chart: enter a formula, name or SMILES to get AXE class, electron and molecular geometry, bond angles, hybridization and polarity in 3D. It is free, works in your web browser and needs no download.

Enter a formula, ion, name or SMILES to get its VSEPR shape. You get the AXE class, steric number, electron and molecular geometry, bond angles, hybridization and polarity, plus a rotatable 3D model with the lone pairs drawn as lobes.

Quick answer: count the atoms bonded to the central atom (X) and its lone pairs (E). NH₃ is AX₃E: 4 electron domains give a tetrahedral electron geometry, but with one lone pair the molecule is **trigonal pyramidal** (107°). Formula, name or SMILES Charge Central atom (SMILES) central atom bonded atoms lone pair Drag to rotate, pinch to zoom

VSEPR chart: all molecular geometries (steric number 2-7)

This chart gives every common VSEPR shape. **X** = atoms bonded to the central atom A, **E** = lone pairs on A. Double and triple bonds count as one domain.

Steric no.	AXE	Bonds	Lone pairs	Electron geometry	Molecular geometry	Ideal angle	Hybrid.	Examples
2	AX ₂	2	0	Linear	Linear	180°	sp	CO ₂ , BeCl ₂
3	AX ₃	3	0	Trigonal planar	Trigonal planar	120°	sp ²	BF ₃ , SO ₃ , NO ₃ ⁻

Steric no.	AXE	Bonds	Lone pairs	Electron geometry	Molecular geometry	Ideal angle	Hybrid.	Examples
3	AX ₂ E	2	1	Trigonal planar	Bent	<120° (≈117°)	sp ²	SO ₂ , O ₃ , NO ₂ ⁻
4	AX ₄	4	0	Tetrahedral	Tetrahedral	109.5°	sp ³	CH ₄ , NH ₄ ⁺ , SO ₄ ²⁻
4	AX ₃ E	3	1	Tetrahedral	Trigonal pyramidal	<109.5° (≈107°)	sp ³	NH ₃ , PCl ₃ , H ₃ O ⁺
4	AX ₂ E ₂	2	2	Tetrahedral	Bent	<109.5° (≈104.5°)	sp ³	H ₂ O, OF ₂ , H ₂ S
5	AX ₅	5	0	Trigonal bipyramidal	Trigonal bipyramidal	90°, 120°, 180°	sp ³ d	PCl ₅ , AsF ₅
5	AX ₄ E	4	1	Trigonal bipyramidal	Seesaw	<90°, <120°	sp ³ d	SF ₄ , TeCl ₄
5	AX ₃ E ₂	3	2	Trigonal bipyramidal	T-shaped	<90°	sp ³ d	ClF ₃ , BrF ₃
5	AX ₂ E ₃	2	3	Trigonal bipyramidal	Linear	180°	sp ³ d	XeF ₂ , I ₃ ⁻
6	AX ₆	6	0	Octahedral	Octahedral	90°, 180°	sp ³ d ²	SF ₆ , PF ₆ ⁻
6	AX ₅ E	5	1	Octahedral	Square pyramidal	<90°	sp ³ d ²	BrF ₅ , IF ₅
6	AX ₄ E ₂	4	2	Octahedral	Square planar	90°	sp ³ d ²	XeF ₄ , ICl ₄ ⁻
7	AX ₇	7	0	Pentagonal bipyramidal	Pentagonal bipyramidal	72°, 90°	sp ³ d ³	IF ₇

Lone pairs always go where they have the most room. In a trigonal bipyramid they sit in the *equatorial* positions (seesaw, T-shaped, linear). In an octahedron, two lone pairs sit opposite each other (square planar).

How to use the VSEPR calculator

1. Type a formula (PCl₅), an ion with its charge (NO₃⁻, SO₄²⁻) or a name (ammonia). For bigger molecules, paste a SMILES string (CC(=O)O) and pick the atom you want to analyse.
2. The tool counts valence electrons and draws the Lewis structure with the same engine as our [Lewis structure generator](#). Then it counts the bonding domains and lone pairs on the central atom.
3. Read the AXE class, electron and molecular geometry, bond angle, hybridization and polarity, with every step shown.

4. Rotate the 3D model to see where the lone pairs (purple lobes) sit and how they squeeze the bond angles.

Worked examples

Water, H_2O (AX_2E_2)

8 valence e^- : 2 O-H bonds + 2 lone pairs = 4 domains (tetrahedral electron geometry).

Bent, 104.5° , sp^3 , polar

Sulfur tetrafluoride, SF_4 (AX_4E)

34 e^- : 4 S-F bonds + 1 lone pair = 5 domains. The lone pair sits equatorial.

Seesaw, sp^3d , polar

Xenon tetrafluoride, XeF_4 (AX_4E_2)

36 e^- : 4 Xe-F bonds + 2 lone pairs opposite each other = 6 domains.

Square planar, 90° , nonpolar

Carbonate, CO_3^{2-} (AX_3)

24 e^- : one C=O and two C-O $^-$ (resonance). 3 domains, no lone pairs on C.

Trigonal planar, 120° , sp^2

VSEPR theory in brief

Valence Shell Electron Pair Repulsion (VSEPR) theory says that the electron domains around a central atom repel each other and spread out as far as possible. A domain is a single, double or triple bond, or a lone pair. The **steric number** (bonded atoms + lone pairs) fixes the **electron geometry**. The positions of the atoms alone give the **molecular geometry**.

Steric number = (atoms bonded to A) + (lone pairs on A)

Repulsion order and bond angles

Repulsion strength runs lone pair-lone pair > lone pair-bond pair > bond pair-bond pair. That is why the angle shrinks from 109.5° (CH_4) to 107° (NH_3) and 104.5° (H_2O). Heavier central atoms show even smaller angles (PH_3 93.5° , H_2S 92°). Multiple bonds also take up more room, which is why the H-C-H angle in formaldehyde is 116.5° rather than 120° .

Named shapes

Trigonal pyramidal: NH_3 , PCl_3 . **Bent:** H_2O (AX_2E_2) or SO_2 (AX_2E). **Seesaw:** SF_4 . **T-shaped:** ClF_3 . **Square pyramidal:** BrF_5 . **Square planar:** XeF_4 . **Trigonal bipyramidal:** PCl_5 . **Octahedral:** SF_6 .

XYZ / Gaussian to 2D Structure Converter

<https://www.moldraw.com/tools/free-chem-tools/xyz-gaussian-to-2d-structure.html>

XYZ and Gaussian file to 2D structure converter by MolDraw. Paste or upload XYZ, Gaussian .gjf, .com, or coordinate text and generate an editable 2D molecular structure canvas with inferred bonds.

In short: Paste or upload XYZ, Gaussian .gjf, .com, or coordinate text and generate an editable 2D molecular structure canvas with inferred bonds. It is free, works in your web browser and needs no download.

Paste or upload XYZ, Gaussian input, or Cartesian coordinate text and generate an editable 2D structure canvas with inferred bonds.

Quick answer: this tool reads atom coordinates, infers likely bonds from covalent radii, projects the 3D geometry into 2D, loads the result into the embedded editor, and exports SVG, PNG, or an inferred MOL file.

Input Coordinates

Upload XYZ / Gaussian file Paste XYZ, Gaussian input, or coordinate block Ready. Paste coordinates and convert.

Editable 2D Structure

Loading editor... Static inferred SVG preview 2D structure preview appears here.

Inferred MOL block

MOL output appears here.

File Format Explained

XYZ stores atom symbols and 3D coordinates, usually without bond orders, charges, aromaticity, or stereochemistry. It is common in computational chemistry and quantum chemistry workflows.

Gaussian input files such as **.gjf** and **.com** often contain a charge/multiplicity line followed by Cartesian coordinates. This tool extracts those coordinate blocks when possible.

Because XYZ and Gaussian coordinate files usually do not store bond order, the output is a best-effort 2D structure. Use the embedded 2D canvas to fix inferred bonds before publication, docking, or downstream cheminformatics.

[SMILES to structure](#) [Structure to SMILES](#) [SMILES to 3D](#) [Mass spectrum predictor](#)

Related chemistry tools

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

XYZ to SMILES Converter | Coordinate File to SMILES

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

XYZ to SMILES converter by MolDraw. Paste or upload an XYZ coordinate file, infer bonds, load the structure into an editable 2D canvas, and copy best-effort SMILES.

In short: Paste or upload an XYZ coordinate file, infer bonds, load the structure into an editable 2D canvas, and copy best-effort SMILES. It is free, works in your web browser and needs no download.

Paste or upload an XYZ coordinate file, infer likely bonds, load the result into an editable 2D canvas, and copy a best-effort SMILES string.

Quick answer: XYZ files do not store bond orders, so this tool builds an inferred MOL file first, lets the MolDraw editor clean the 2D layout, and then reads SMILES from the editable structure.

Input XYZ Coordinates

Upload XYZ file Paste XYZ text Ready. Paste XYZ coordinates and convert.

SMILES Output and Editable Structure

Loading editor... Generated SMILES [Open SMILES in MolDraw](#)

Inferred MOL block

Input and output formats

Input: XYZ coordinate file	Output: SMILES	
Full name	XYZ coordinate file	SMILES (Simplified Molecular Input Line Entry System)
What it holds	Element symbols and x, y, z coordinates only. Bonds are not stored and must be worked out.	Atoms, bonds, rings, charges and stereo as one line of text. No coordinates.
File or form	.xyz	.smi or plain text

XYZ to SMILES Notes

XYZ files normally store atom symbols and 3D coordinates only. They usually do not include bond orders, formal charges, aromaticity, or stereochemistry.

Use this as a best-effort converter. Review the inferred bonds in the 2D editor before using the SMILES in databases, modeling tools, publications, or assignments.

- Carbon-bound hydrogens are hidden before SMILES generation so the editor can use normal implicit hydrogens.
- Bond orders are inferred as single bonds; fix double bonds, aromatic rings, charges, and stereochemistry manually when needed.

- For a visual editable structure first, use the [XYZ / Gaussian to 2D Structure converter](#).

[XYZ / Gaussian to 2D structure](#) [Structure to SMILES](#) [SMILES to structure](#) [SMILES to 3D](#)

Related chemistry tools

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