# Aufbau

*Chemistry, computed from first principles*

*User's Guide*

Version 1.0 · macOS · aufbau.app

# Contents

# 1. What Aufbau is

*Aufbau shows why chemistry happens. Every result — a bond that forms, an orbital's shape, an infrared band, a reaction that runs or refuses to — is* ***computed from the model in real time****, not looked up in a table and not scripted for a nicer story. If the engine can't compute something honestly, the app says so rather than inventing an answer.*

That single idea shapes the whole app. Reactions resolve to their lowest-energy bonding arrangement from electronegativity, valence, and activation energy. Geometry comes from VSEPR and real covalent radii. Spectra are read off the same bond graph the reactor produces. Nothing is faked, and nothing is stored as a pre-computed "right answer."

Aufbau is built for undergraduate and advanced high-school chemistry — general through introductory organic — plus a nuclear-chemistry module. It's for instructors who want to show the mechanism, and students who want to see it.

# 2. Getting started

Aufbau opens on the **periodic table**. Select any element from the list to see its electron shells, orbital configuration, and oxidation states in the detail pane. Use the search field to jump straight to a symbol.

## The Tools menu

Everything else lives under the **Tools** menu (the grid icon in the toolbar). Each tool opens in its own space so you can focus on one idea at a time:

- **Chemistry Workbench** — build your own reactions and let the engine judge them.
- **Reaction Lab** — a live reactor where molecules collide, bond, and settle.
- **Reactor (3-D)**, **Molecule Shapes**, **Design** — structure and geometry.
- **Nuclear** and **Carbon Under Pressure** — transmutation and phase behavior.
- **Radical Qubits**, **Spin-Qubit Dynamics**, **Entanglement Lab**, **Diamond NV Qubit** — the quantum side.
- **Proton NMR** and **IR Normal Modes** — spectroscopy from the bond graph.
- **Explore Element** and **Configuration Filter** — go beyond the known table.

# 3. Chemistry Workbench

*The Workbench is where you compose a mixture and ask the engine whether it reacts. It gives an honest verdict — a favourable product forms, or it doesn't — and lets you save either outcome to revisit later.*

## Building a mixture

On the **Build** tab, add reagents three ways: tap a molecule or single atom from the palettes; type a formula or a SMILES string by hand; or pull from the **Reagent Shelf** — a stockroom of 26 common reagents (acids, bases, oxidizers, gases, organics, salts), each shown with its real structure. Use the –/+ steppers to set how many of each.

## Reacting and reading the result

Tap **Test**. A green "Reacts" banner shows the products and the change in bonding energy; an amber verdict means nothing favourable formed. When several products form, the blue **Product** pill lets you choose which one to focus on — the SMILES, the proton-NMR read-out, the 3-D view, retrosynthesis, and orbitals all follow your choice.

## Saving and recalling

Name the reaction and save it to your working library (or a "to refine" shelf for ideas that didn't pan out). Everything is stored on your device — recall, rename, or delete from the **Saved** tab. You can also send a mixture straight to the Reaction Lab with **Run in Reaction Lab**.

# 4. Reaction Lab

*The Reaction Lab is the reactor running live: reactant molecules share a box, interact all at once, and settle into products — the engine's own chemistry deciding which reactions fire.*

## Two views

- **Live** — watch atoms drift, collide, bond, and reform as a scene.
- **Ledger** — the same reaction as a running account of what formed and broke.

## Driving the reaction

Use the temperature slider, or the quick **Cool down** / **Heat pulse** buttons, to push the mixture over (or under) its activation barriers. **Reset** reseeds the starting mixture. **Breathe** cycles the temperature so a reversible binding — oxygen onto heme, for example — visibly comes and goes.

## See in 3-D & Energy

**See in 3-D** opens the products as real structures you can rotate. **Energy** shows the reaction's energy profile — reactants, the activation hump, products — computed from the engine's own bond-strength function.

## Water-splitting & energy sources

The water-splitting scenario models the real thermodynamic bill: un-burning water costs energy, so it only runs while there's budget. Flip on **Solar** or **Thorium** to pour energy in from outside and watch the catalytic cycle run cleanly — a first-law lesson you can see.

# 5. Seeing structures in 3-D

Any product or entered molecule can be rendered as a real three-dimensional structure. Simple molecules use a crisp VSEPR layout; everything else — metal complexes, big rings — is laid out from its actual bond graph using true covalent bond lengths, so a metal–ligand bond renders genuinely longer than a C–H bond, because it really is.

Rotate with a drag, tap an atom to identify it, and toggle between reactants and products. Aromatic rings carry a translucent π-cloud; metal clusters show their shared electron sea.

# 6. Spectra — IR & NMR

*Spectra in Aufbau are a view of the bond graph, computed — never stored.*

**IR Normal Modes** builds the mass-weighted Hessian and diagonalises it, so the bonds' motions mix into true normal modes. The translation/rotation modes fall to zero on their own — nothing enforces that; it happens only if the physics is right.

**Proton NMR** reads the hydrogen environments straight off the structure — shifts, multiplicities, and integrations, all from connectivity, with no stored spectrum.

# 7. Orbitals, spin & qubits

For H/C/N/O molecules, Aufbau computes molecular orbitals with an extended-Hückel treatment and draws the HOMO/LUMO and spin density as real wavefunction lobes and smooth isosurfaces. Where the engine can’t solve a molecule (for example one containing a metal), it says so rather than drawing a fake picture.

The quantum tools — **Radical Qubits**, **Spin-Qubit Dynamics**, **Entanglement Lab**, and the **Diamond NV Qubit** — carry the same idea into spin: unpaired electrons as qubits, and a nitrogen-vacancy centre you read with light (its ODMR dips slide apart as you sweep a magnetic field).

# 8. Nuclear & matter under pressure

The **Nuclear** module steps outside ordinary chemistry to change the nucleus itself — decay, transmutation, and breeding chains — the physics that lets thorium power the water-splitter in the Reaction Lab.

**Carbon Under Pressure** shows Le Châtelier by molar volume: squeeze graphite and its Gibbs energy falls until diamond wins — straight from $\Delta G° + \Delta V \cdot \Delta P$, with the crossover pressure computed live as you turn the dials.

# 9. Exploring the periodic table

Beyond the known elements, **Explore Element** lets you ask for a hypothetical element by proton count and see its predicted configuration, and **Configuration Filter** answers natural-language queries about the table (“all noble elements up to proton count 797”). It’s a way to probe the logic of the aufbau principle the app is named for.

# 10. Privacy

Aufbau runs **entirely on your device**. It collects nothing, has no accounts or analytics, and makes no network connections. Your saved reactions live in the app’s own container and never leave your Mac. Full details are on the Privacy page at aufbau.app.

# 11. About & credits

Aufbau is made by **AppProved Software Corporation**. Its computational-chemistry approach traces back to the LHASA computer-assisted-synthesis lineage — work its author contributed to (Corey, Long, Greene, Miller, *J. Org. Chem.* **1985**, *50*, 1920).

The name honours the **aufbau principle**: build up from the ground state, one electron at a time. That is how the app works, too — everything computed from first principles.

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