Chemora
LOGIDFT

HARI GROUP

LogiDFT - How to Use

From Gaussian log files to Supporting-Information text, 3D structures and a balanced, branched reaction energy profile - worked through with the demo data.

> **What the tool does.** Every structure's final energy is **G = HF (single-point log) + thermal correction to Gibbs free energy (frequency log)**. For relative ΔG and the energy profile, every stage is balanced so it has the **same atoms and the same number of electrons** as the reference stage, by adding or subtracting the energy of reagents / by-products (balancing species). Stages can be connected in any order, including branched paths.

What you need

• A **frequency** log (opt+freq or freq) for every structure - thermal corrections and number of imaginary frequencies.
• A **single-point (sp)** log for the same geometry at the higher level of theory - the HF/SCF energy. Name it like the frequency file plus `_sp`: `Int-I.log` + `Int-I_sp.log`. Matching geometry also pairs them.
• The demo files: click **Demo log files** in the upload box (`LogiDFT_demo_logs.zip`), unzip, and follow along - 6 structures x (freq + sp) = 12 files.
• **Your data stays private:** click the pulsing **info icon** in the top-right of the banner. Files are parsed locally in your browser - nothing is uploaded.

The demo reaction

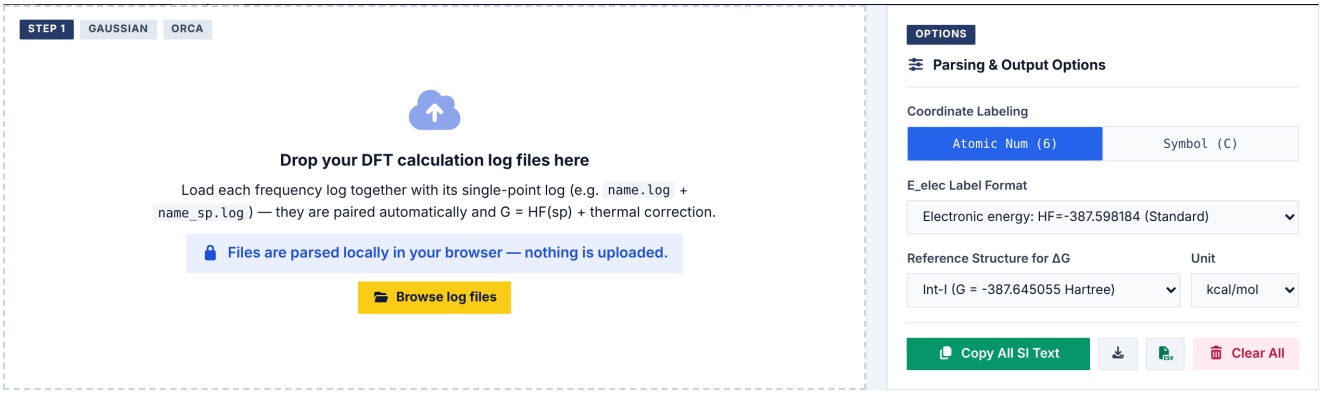
Stage	Atoms	Role
Int-I	C5 (30 e-)	Reference stage
TS-1, TS-2	C5	Transition states (1 imaginary freq.)
Int-II	C5	Intermediate
Product	C3 (18 e-)	Lost two carbons - needs balancing
Reagent-B	C2 (12 e-)	Balancing species (the lost C2)

Buttons in the top-right of the banner

Button	What it does
Expand icon	Full-screen mode (see Step 7): hides the site header, banner and footer.
How to Use?	Opens this guide.
Info icon (pulsing)	Privacy note: files are processed locally, nothing is uploaded.
Moon / sun icon	Switches between light and dark theme.

Step 1 - Load the log files

Drop all files on the page, or click **Browse log files** (multi-select is fine). Parsing is done locally in your browser. Load them in the order you want the stages to appear: Int-I, TS-1, Int-II, TS-2, Product, Reagent-B (freq + sp for each); you can reorder later by dragging.

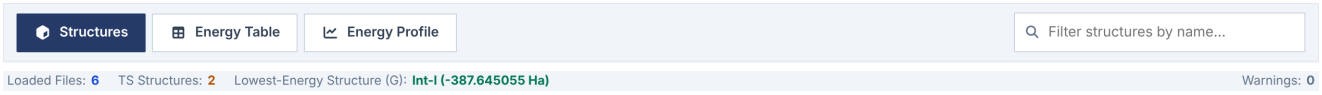


Upload box and Parsing & Output Options: coordinate labeling (atomic number or symbol), E_elec label format, the reference structure for ΔG, and the energy unit.

A message confirms the pairing, e.g. "*Processed 12 log file(s) -> 6 structure(s), 6 with freq + sp paired.*" If a structure shows **No sp log paired** its energy comes from the frequency job - add the matching sp file.

The tab bar and summary line

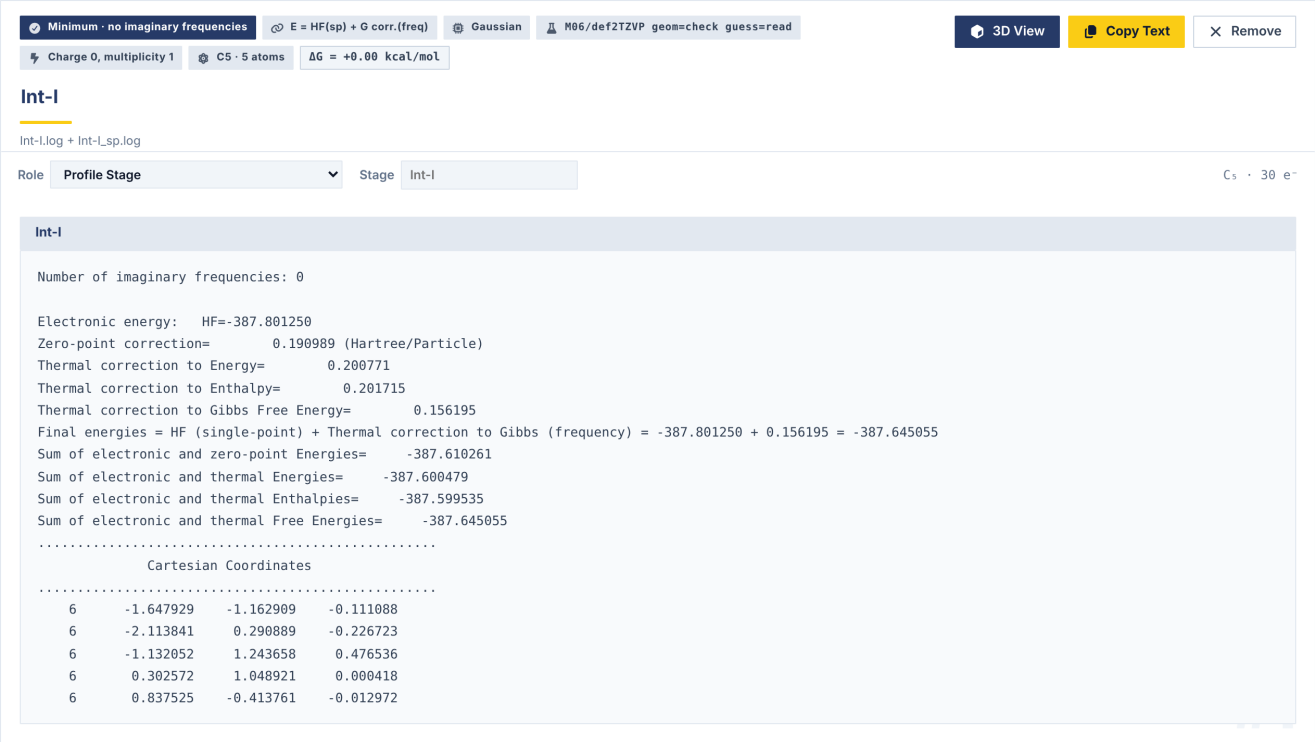
Directly under the upload box and options, one grey bar holds the three views - **Structures**, **Energy Table**, **Energy Profile** - and, on the Structures tab, the **filter-by-name** box. The bar sticks to the top while you scroll, and a **Copy All SI Text** button appears in it. Just below it a small summary line shows the number of loaded files, TS structures, the lowest-energy structure and warnings.



Step 2 - Check each structure

Each structure gets a card. The tags at the top show **Minimum / Transition state** (dark blue), the pairing (**E = HF(sp) + G corr.(freq)**), program, level of theory, charge/multiplicity, formula and the relative ΔG. The three buttons - **3D View**, **Copy Text**, **Remove** - are at the top right of the card; click the title to rename the structure. The text block is ready to paste into Supporting Information and ends the energy section with the final energy:

```
Final energies = HF (single-point) + Thermal correction to Gibbs (frequency) = -387.801250 + 0.156195 = -387.645055
```



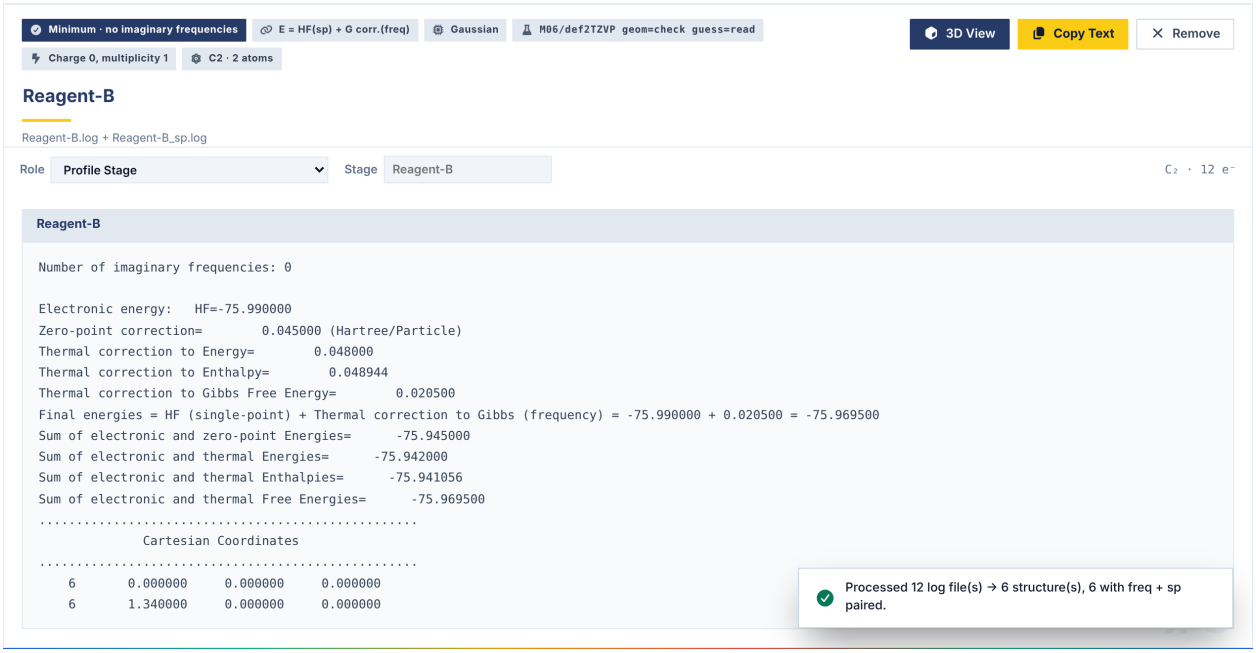
Card for Int-I. **3D View** opens the structure, **Copy Text** copies the SI block, **Remove** deletes the file. Use the filter box in the tab bar and the Sort menu below it to find structures; the toolbar also opens or closes all 3D views.

3D viewer

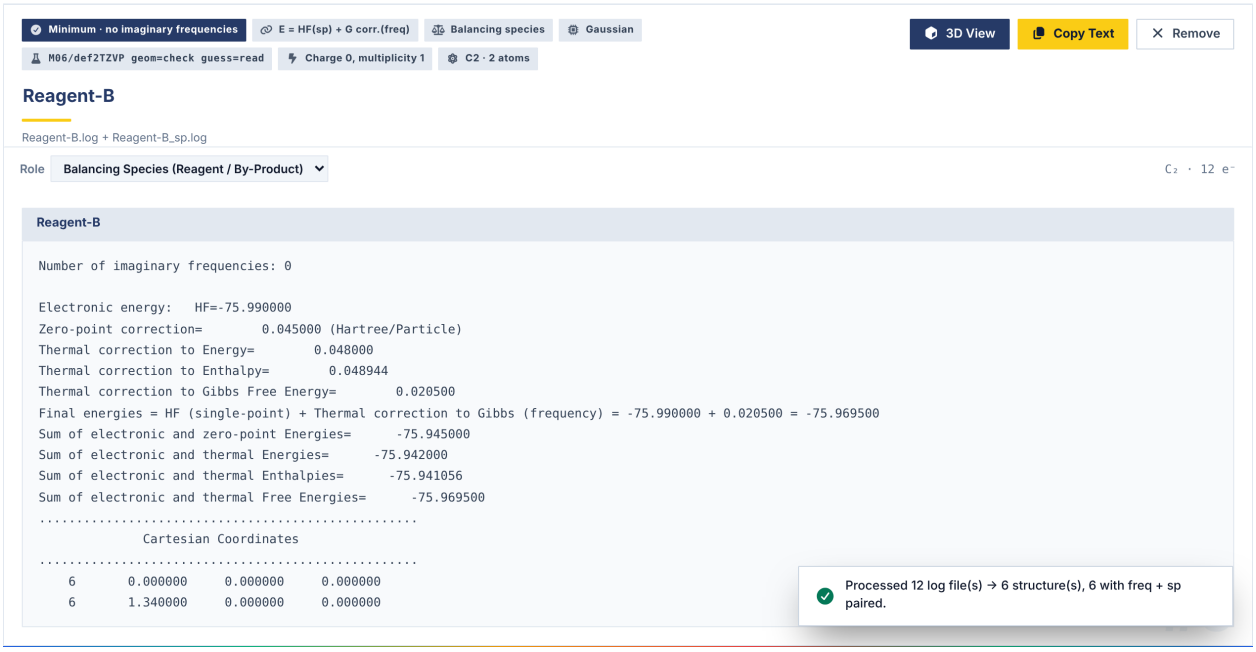
Ball-and-stick on a white background (C gray, H white, N blue, O red, Ni green, B pink). Atoms in the back fade out automatically. Drag to rotate, scroll to zoom. Styles: Ball & Stick, Stick, Spacefill, Wire. Labels, hide H, measure distances/angles, auto-spin, **Animate TS Mode** for the imaginary vibration, PNG and XYZ export.

Step 3 - Balance atoms and electrons

In the demo, Product is C3 (18 electrons) but the reference Int-I is C5 (30 electrons). The missing C2 (12 electrons) is Reagent-B. On the **Reagent-B** card, change **Role** from *Profile Stage* to *Balancing Species*:



Before: Reagent-B is treated as a profile stage.



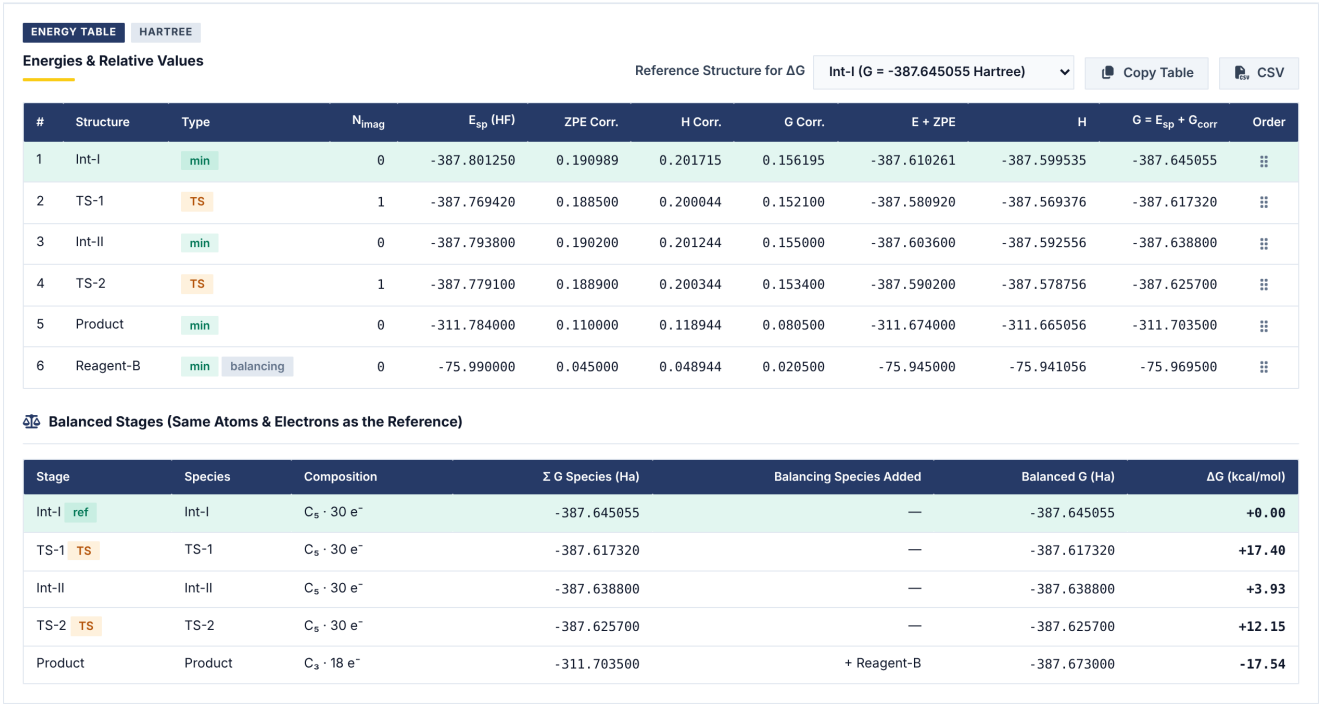
After: Reagent-B is a balancing species (the Stage box disappears).

Several species in one stage? Type the same **Stage** label on each card (e.g. catalyst + substrate -> "Int-I"); their energies are summed. **Which species balance?** Anything that enters or leaves the profile - reagents, ligands, water, by-products. The tool finds the smallest whole-number combination (e.g. + *Reagent-B* or - *2 x Water*) that makes atoms and charge equal to the reference.

Step 4 - Energy Table

Open the **Energy Table** tab. The upper table lists every species (E(sp), corrections, G). The lower **Balanced Stages** table shows, per stage, the composition, the balancing species added or removed, the balanced G and the final ΔG. Use the **Reference Structure for ΔG** dropdown next to **Copy Table** and **CSV** to change the zero of the scale.

Reorder by dragging: grab the grip handle in the **Order** column and drag a row up or down - the other rows slide out of the way. (With the handle focused, the up/down arrow keys also work.) The order sets the order of the stages in the profile.



ENERGY TABLE HARTREE

Energies & Relative Values

Reference Structure for ΔG: Int-I (G = -387.645055 Hartree) | Copy Table | CSV

#	Structure	Type	N_{imag}	E_{sp} (HF)	ZPE Corr.	H Corr.	G Corr.	E + ZPE	H	$G = E_{sp} + G_{corr}$	Order
1	Int-I	min	0	-387.801250	0.190989	0.201715	0.156195	-387.610261	-387.599535	-387.645055	
2	TS-1	TS	1	-387.769420	0.188500	0.200044	0.152100	-387.580920	-387.569376	-387.617320	
3	Int-II	min	0	-387.793800	0.190200	0.201244	0.155000	-387.603600	-387.592556	-387.638800	
4	TS-2	TS	1	-387.779100	0.188900	0.200344	0.153400	-387.590200	-387.578756	-387.625700	
5	Product	min	0	-311.784000	0.110000	0.118944	0.080500	-311.674000	-311.665056	-311.703500	
6	Reagent-B	min balancing	0	-75.990000	0.045000	0.048944	0.020500	-75.945000	-75.941056	-75.969500	

Balanced Stages (Same Atoms & Electrons as the Reference)

Stage	Species	Composition	Σ G Species (Ha)	Balancing Species Added	Balanced G (Ha)	ΔG (kcal/mol)
Int-I ref	Int-I	$C_5 \cdot 30\ e^-$	-387.645055	—	-387.645055	+0.00
TS-1 TS	TS-1	$C_5 \cdot 30\ e^-$	-387.617320	—	-387.617320	+17.40
Int-II	Int-II	$C_5 \cdot 30\ e^-$	-387.638800	—	-387.638800	+3.93
TS-2 TS	TS-2	$C_5 \cdot 30\ e^-$	-387.625700	—	-387.625700	+12.15
Product	Product	$C_3 \cdot 18\ e^-$	-311.703500	+ Reagent-B	-387.673000	-17.54

Product: C3 + Reagent-B (C2) = C5, 30 electrons, same as Int-I. ΔG = G(Product) + G(Reagent-B) - G(Int-I).

Step 5 - Energy Profile

The **Energy Profile** tab plots the balanced stages as dots joined by smooth curves; transition states are orange. Top row: **Energy** type (G, H, E0, E), **Line Style** (default for all lines), **Grid Lines**, **Show Values**. **Save SVG / Save PNG** export a white-background figure for papers and slides - your appearance choices are included.

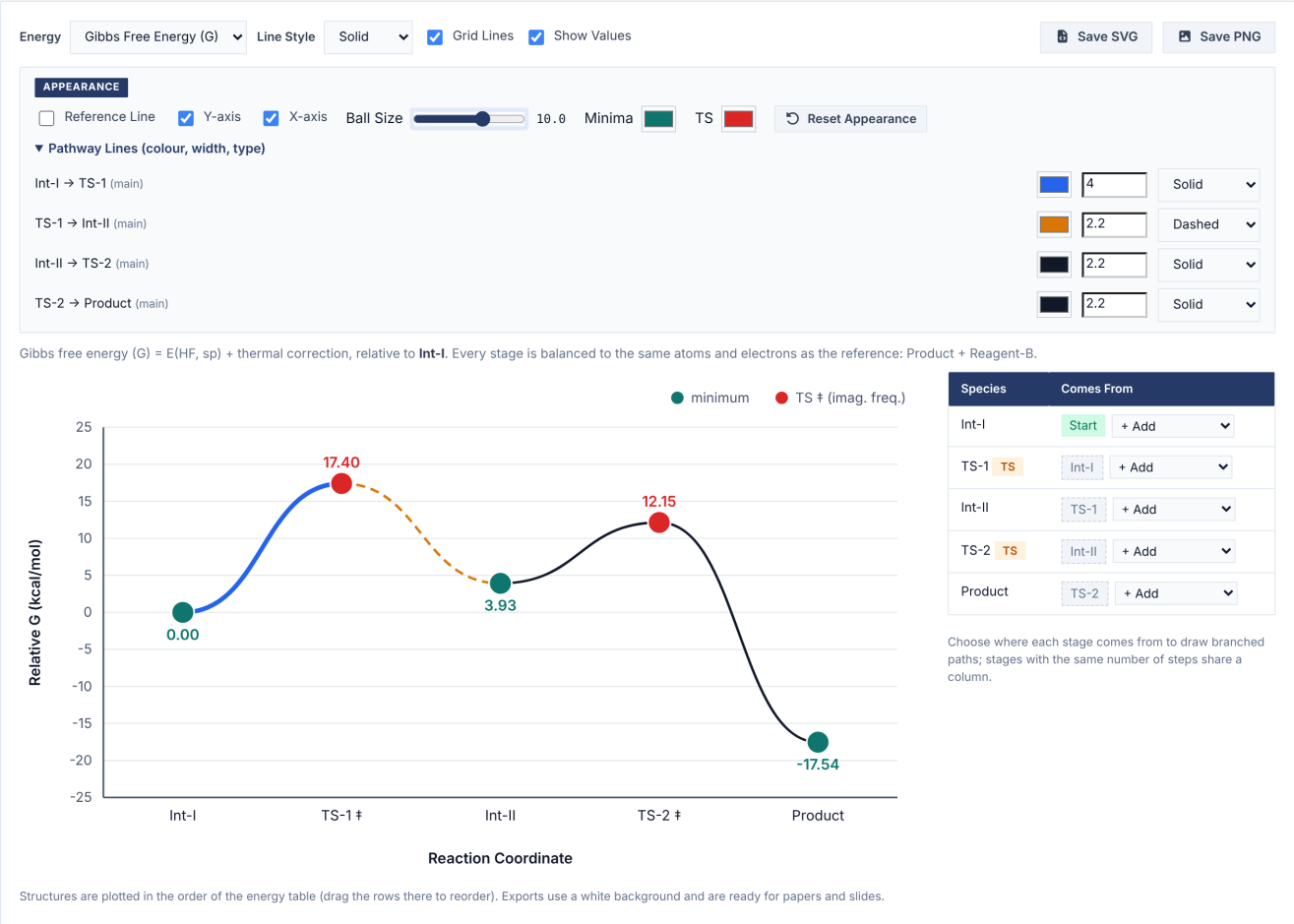


Default profile with the Appearance panel: each stage comes from the previous one. The table on the right lists every plotted species and where it comes from.

Step 5b - Customise the profile (Appearance panel)

The **Appearance** panel above the chart controls how the figure looks. Changes apply instantly and are used in the SVG / PNG export.

• **Reference Line / Y-axis / X-axis** - tick boxes switch the dashed zero (reference) line and each axis on or off. Switching an axis off hides its line, tick or stage labels and its title.
• **Ball Size** - slider (3-14) for the size of every point on the profile.
• **Minima / TS** - colour pickers for the balls of minima and transition states (the legend follows).
• **Pathway Lines** - open the drop-down to see every line, named by the two stages it joins (e.g. *Int-I -> TS-1*). For each one choose its **colour**, **width** (0.5-8) and **type** (solid, dashed, dotted).
• **Reset Appearance** restores all defaults.



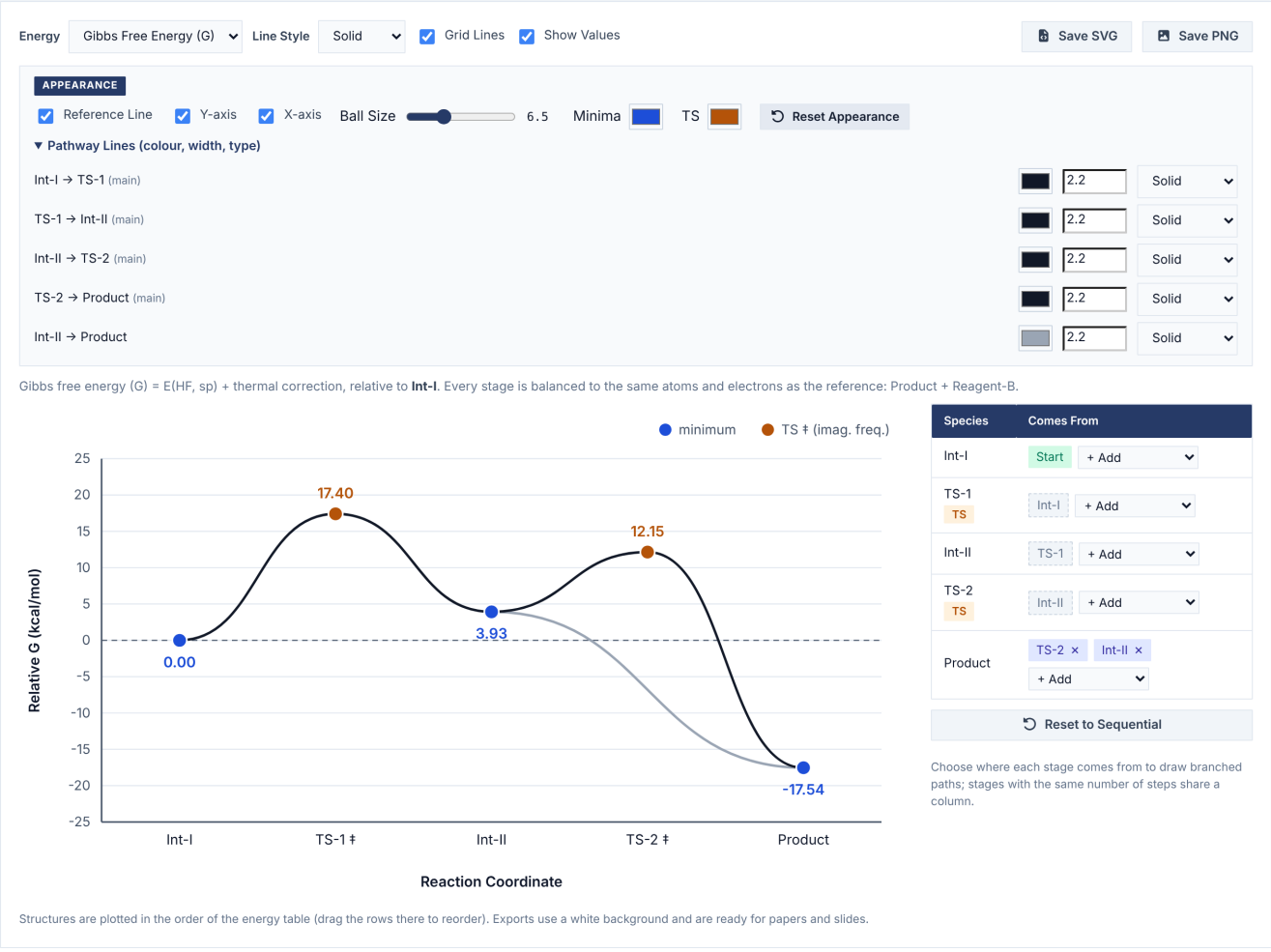
Example: reference line off, larger green / red balls, first path thick blue, second path dashed orange.

Remembered: the on/off choices, ball size and ball colours are saved in your browser. Per-line styles and the *Comes From* choices are not saved when you reload the page.

Step 6 - Branched paths with "Comes From"

Real mechanisms branch. In the table beside the profile, each species has a **Comes From** cell:

• By default it shows the previous stage (dashed chip).
• Pick another stage from **+ Add** to add a connection - a species can come from several stages. Click **x** on a chip to remove one; **Start (no parent)** makes a species a starting point.
• Every connection is drawn as a smooth curve. The first path from a stage is **black**, extra branches are **grey** (their colour, width and type can be changed in the Appearance panel). Stages with the same number of steps from the start share a column.
• **Reset to Sequential** restores the default chain.

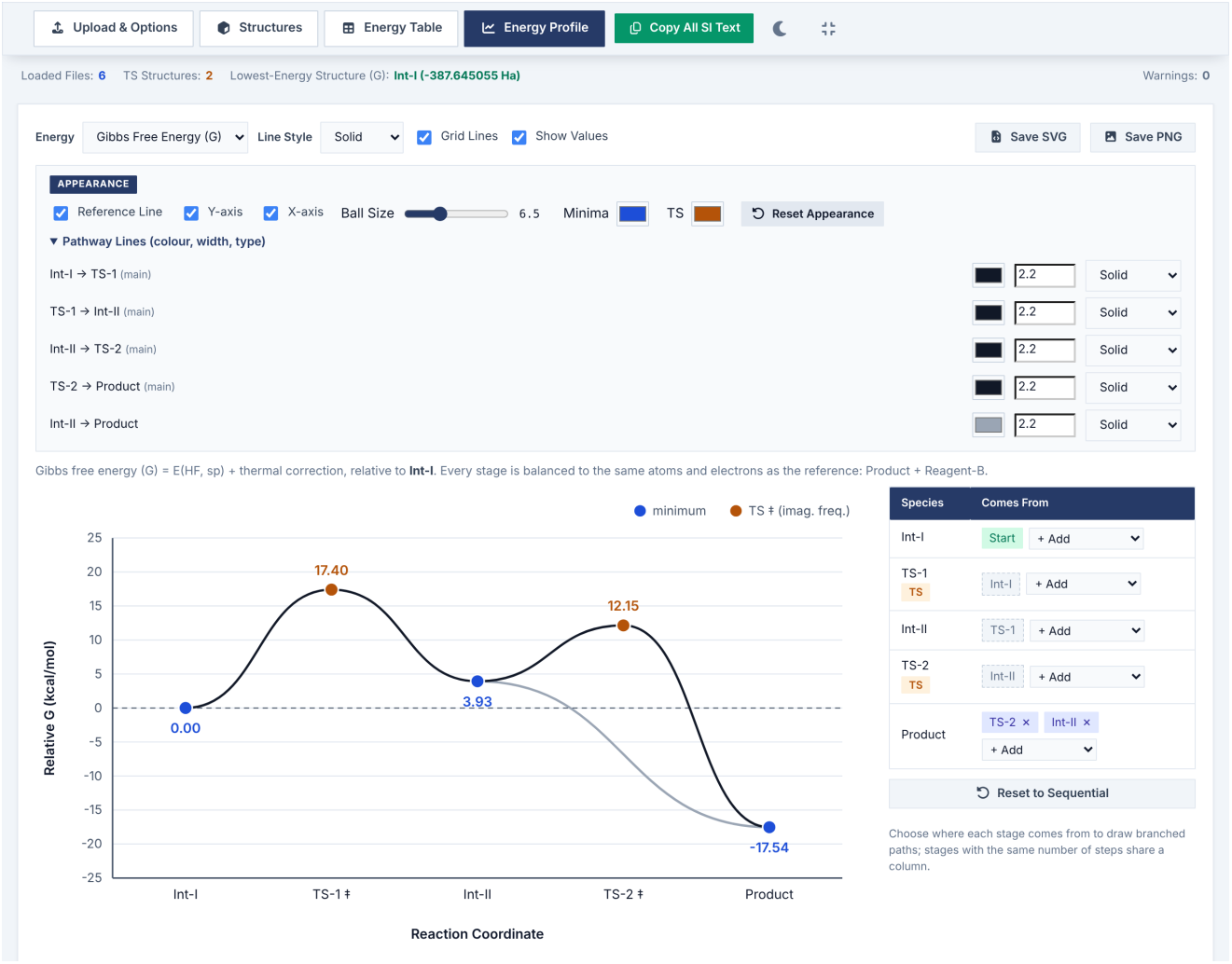


Here Product comes from TS-2 (main path) and also directly from Int-II (grey branch).

Example from a real study: if an intermediate leads both to a second transition state and to a side product, set the side product's **Comes From** to that intermediate - it appears as a grey branch ending at the side product. The "Comes From" choices are not saved when you reload the page.

Step 7 - Full-screen mode

Click the **expand icon** just before **How to Use?** in the banner. The site header, banner and footer disappear and the tool fills the screen. All tools are tabs in the top bar: **Upload & Options**, **Structures**, **Energy Table**, **Energy Profile**, plus **Copy All SI Text**, the theme toggle and the **minimize icon**. Click the minimize icon (or press Esc) to return to the normal page.



Full-screen mode showing the Energy Profile tab.

Exports

- **Copy All SI Text** / **Download**: SI text for every structure; **CSV** or **Copy Table**: the energy tables.
- Per structure: **Copy Text**, XYZ coordinates, PNG of the 3D view.
- Profile: **Save SVG** / **Save PNG** (with your Appearance settings).

Troubleshooting

Message / symptom	What to do
No sp log paired	Add the single-point log (name_sp.log), or make sure both logs have the same geometry.
Stage "cannot be balanced"	Load the missing reagent/by-product (freq + sp) and set it to Balancing Species.
"missing energy"	A stage member lacks the sp or the frequency log (thermal correction).
Charge/multiplicity or geometry differ	The freq and sp logs are not for the same species - check the files.
A stage is far off (hundreds of kcal/mol)	Usually the sp log is at a different level of theory or not the matching geometry - check the pairing.
More than 1 imaginary frequency	Higher-order saddle point - re-optimise the structure.
3D view empty	Check the internet connection (3Dmol.js loads from the web) and reload.