

# ACE Mechanism Calculator

<http://aceorganic.pearsoncmg.com/epoch-plugin/public/mechmarvin.jsp>

The ACE mechanism calculator is an excellent way to check your curved arrows. Paste your structure into the MarvinSketch window and click on View Products. The result will be shown in the MarvinSketch window and the overall chemical equation will be shown at the top.

**ACE mechanism calculator**

Draw a mechanistic step involving one or more compounds and electron-flow arrows, and press **View Products** to calculate the products.

**ACE mechanism calculator**

Draw another mechanistic step involving one or more compounds and electron-flow arrows again! [Note: A criss-cross bond indicates a broken bond.]

**Overall chemical equation**

The image displays the ACE mechanism calculator interface. At the top, there are two panels. The left panel shows the input step: a protonated amine (N<sup>+</sup>H<sub>3</sub>) reacting with water (H<sub>2</sub>O). A curved arrow indicates the lone pair on the nitrogen atom attacking a proton on the water molecule. The right panel shows the overall chemical equation: the protonated amine + water → the neutral amine + a hydronium ion (H<sub>3</sub>O<sup>+</sup>). Below these panels are two MarvinSketch windows. The left window shows the input step with a 'View Products' button highlighted. The right window shows the resulting products: the neutral amine and the hydronium ion. A large blue arrow points from the 'View Products' button in the left window to the overall chemical equation. A QR code is located in the bottom right corner.

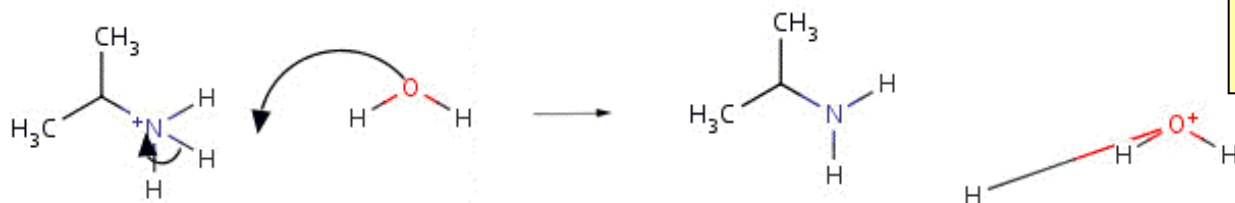
**products**

View Source (MOL) View Source (MRV)

# Make the Results Look Nice - Clean in 2D

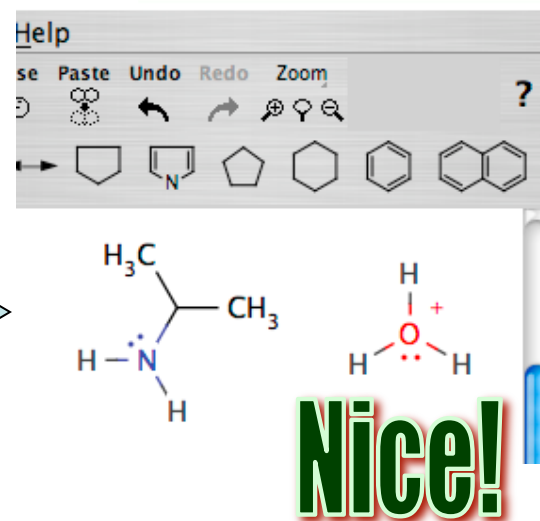
## ACE mechanism calculator

Draw another mechanistic step involving the calculated products or one or more other compounds, and try it again! [Note: A criss-cross bond indicates a double bond with indeterminate stereochemistry.]



The mechanism calculator will produce some funky looking structures. Sometimes the results can be difficult to discern. Use this procedure to clean up the result.

Software interface showing the 'Clean' menu path: **Clean** > **2D** > **Clean in 2D**. The 'Clean in 2D' option is selected, and a sub-menu offers: No optimization,  Optimize if needed, Optimize, and Wedge bonds. A blue arrow points from the 'Clean in 2D' menu to the resulting clean 2D structures.



# Make Friends with MarvinSketch

## MarvinSketch Quick Help

<http://aceorganic.pearsoncmg.com/nosession/marvin/chemaxon/marvin/help/sketch.html>

### Keyboard shortcuts

- All the elements. For example: **N** is Nitrogen, **Cl** is Chlorine etc. (Also works in lower case: **n**, **cl** etc.)
- Query atom types: **\*** (any atom), **Q** (heteroatom), **R-groups**: **R1**, ..., **R32767**. (Also in lower case.)
- Atom maps for reactions: **M1**, **M2**, ..., **M+** (next unused mapping number), Unmap: **M0**. (Also in lower case.)
- Bond types: **1**, **2**, **3**, **4** (aromatic), **1-2** (single or double), **1-4** (single or aromatic), **2-4** (double or aromatic), **0** (any)
- Charges: **-**, **+**
- Stereochemical groups: **abs** (ABSOLUTE), **or1**, **or2**, ..., **or10**, ... (OR *n*), **and1**, **and2**, ..., **and10**, ..., **&1**, **&2**, ..., **&10**, ... (AND *n*)
- Abbreviated groups: **Ph** = Phenyl, **Ala** = Alanyl, etc. (Also in lower case.)  
To complete a longer name, press **Enter** or **End** after typing the first few characters.
- Templates: **1-1**, **2-2**, ... **9-9**
- Special atom properties: **.a** (aromatic), **.A** (aliphatic), **.u** (unsaturated), **.H0**, **.H1**, ... (number of hydrogens), **.h0**, **.h1**, ... (implicit hydrogens), **.X0**, **.X1**, ... (connectivity), **.D0**, **.D1**, ... (degree), **.R0**, **.R1**, ... (rings), **.r3**, **.r4**, ... (smallest ring size), **.s\***, **.s0**, **.s1**, ... (substitution count), **.v0**, **.v1**, ... (valence), **.rb\***, **.rb0**, **.rb1**, ... (ring bond count).
- More window (Periodic Table): **Ctrl-M**
- Undo: **Ctrl-Z**, **Alt-Backspace**, Redo: **Ctrl-Y**
- Clipboard. Copy: **Ctrl-C**, Copy as Smiles: **Ctrl-L**, Cut: **Ctrl-X**, Paste: **Ctrl-V**, Select all: **Ctrl-A**
- File operations (if available). Open: **Ctrl-O**, Save: **Ctrl-S**, Print: **Ctrl-P**
- To define a set of fragments as **R-group** **5**: select the fragments, then type **R-5**.
- To choose an attachment point on **R-group** **5**: type **R-5**, then click on the atom.

**experiment!**