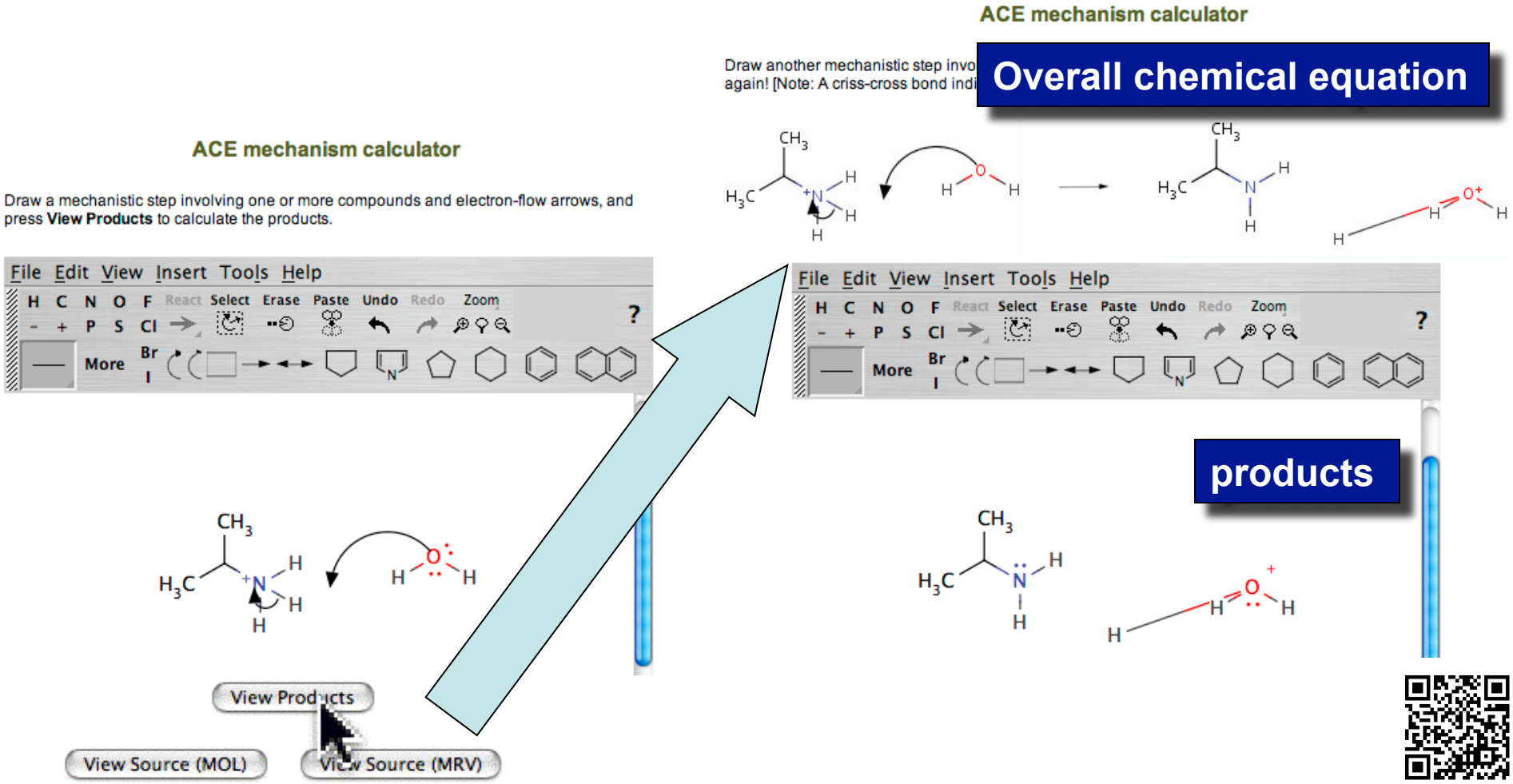
ACE Mechanism Calculator

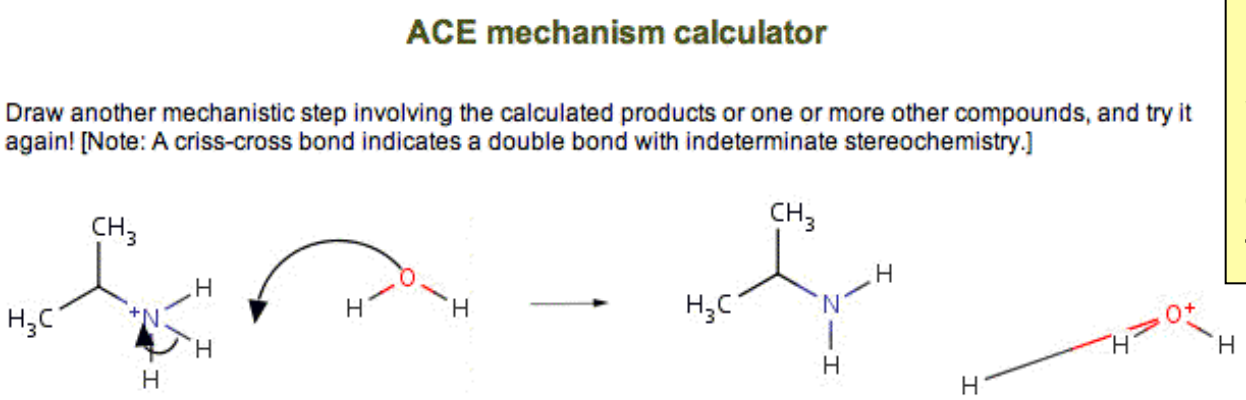
http://aceorganic.pearsoncmg.com/epoch-plugin/public/mechmarvin.jsp

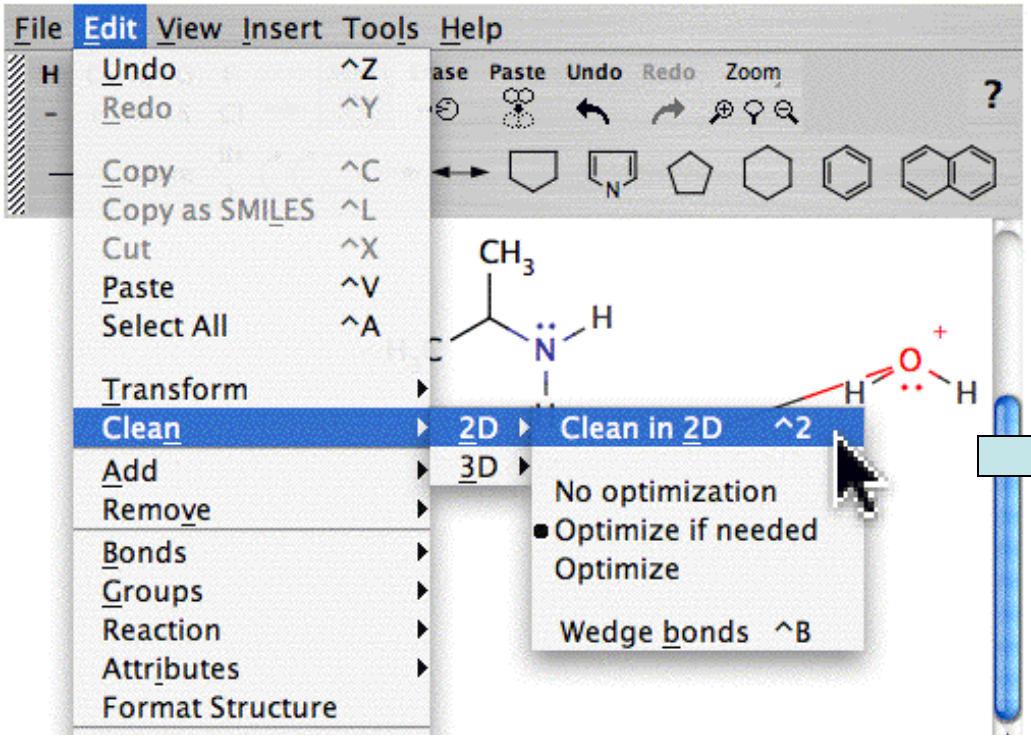
The ACE mechanism calculator is an excellent way to check your curved arrows. Paste your structure into the MarvinSketch window and click on View Products. The result will be shown in the MarvinSketch window and the overall chemical equation will be shown at the top.

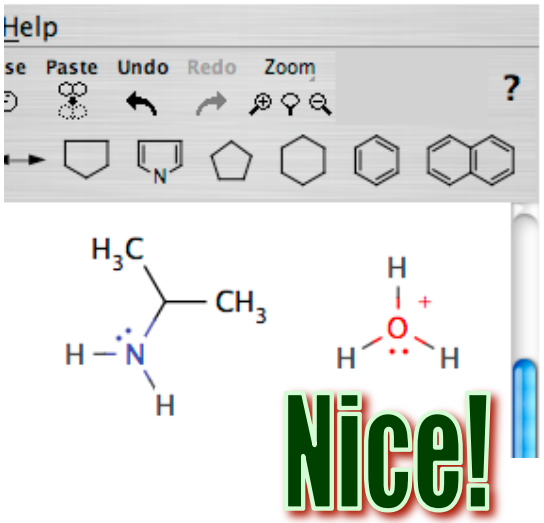


Make the Results Look Nice - Clean in 2D

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.







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.