There's something about eChem

- ✓ What is eChem? What can eChem do for me?
- ✓ Are there any system requirements to run eChem?
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- ✓ How can I **construct** a molecular model?
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- ✓ How can I **analyze** chemical/physical properties base on molecular structures?

✓ *What is eChem? What can eChem do for me?*

eChem is a chemistry software package for you to create virtual three-dimensional models of molecules, simultaneously visualize multiple representations of molecules, and compare properties of molecules. eChem includes three main actions: Construct, Visualize and Analyze.
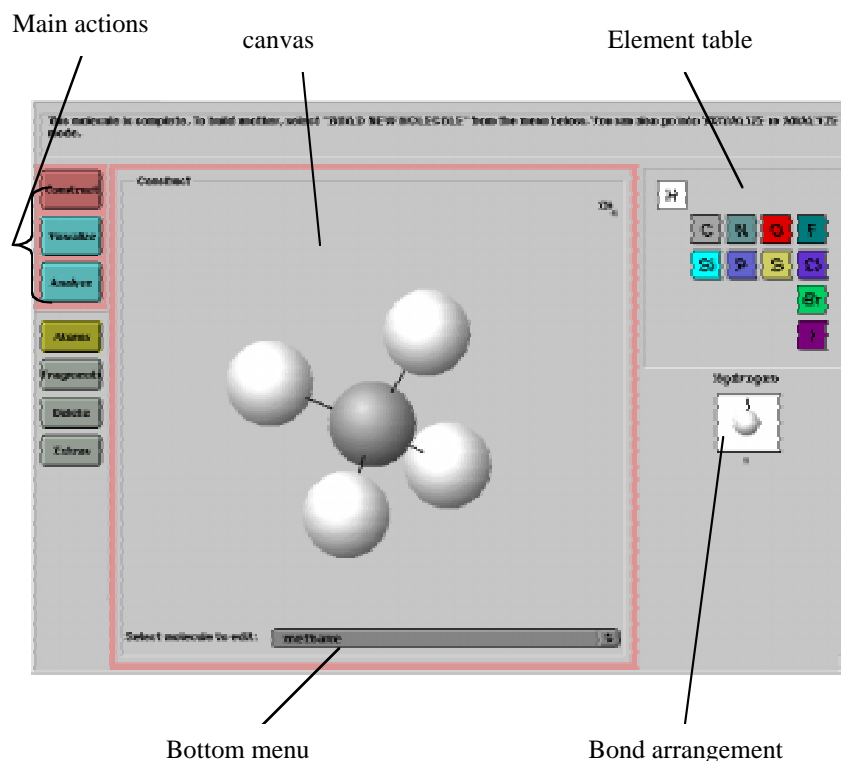
✓ *Are there any system requirements to run eChem?*

There are two versions of eChem now, which can run on Mac and IBM machines.

	Macintosh	IBM-compatible
Web version	Internet Explorer 4.0[a]	Internet Explorer 4.0[b]
Application version	Mac OS 8.0 (or later) and MRJ 2.0[c]	Windows version requires Internet Explorer 4.0 (with the Microsoft VM) and the latest Java patches/updates.

a. Compared with running on IBM-compatible machines, eChem web version runs relatively slow on Mac, even though it's on a Power G3. Thus Application version is highly recommended.

b. Netscape 4.05 does not provide Java support for running eChem.

c. The full name of MRJ is Mac OS Runtime for Java. It is free software and downloaded from
http://develop.apple.com/java/index.html

✓ *How can I get eChem? Can I use it at home?*

You can get both web and application versions of eChem at
http://kermit.eecs.umich.edu/html/echem

Main actions   canvas   Element table

Bottom menu   Bond arrangement

✓ *How can I **construct** a molecular model?*

<mark>To construct the model of methane (CH4), start on the left side of the screen, when you see "Construct", "Visualize" and "Analyze".</mark>

c1. Click "Construct"

c2. A small window jumps up. Enter the name of molecule: methane.

c3. Click "Atoms", and select "C" (carbon) from element table on the right side of the screen.

c4. Select bond arrangement. In this case, select "tetrahedral" as the hybridization of carbon and click on the canvas (the large screen in the middle).

c5. Select "H" from atom table and select hybridization.

c6. Add hydrogens to the carbon's bond by clicking on the bonds of carbon. (Here is an easy way to attach all hydrogen atoms by one click. Select "extras" feature in the "construct" window. Click "fill in hydrogens.")

c7. You can see a rotating structure; just hold down the mouse button, and move the cursor.

c8. How can you save this methane model? Go to menu bar "file" and select "save." Input the file name as "methane.alc" (remember to add ".alc" after the compound's name or you can't open the file next time)

c9. Did you attach a wrong atom on carbon (like adding an oxygen atom for methane)? Select "Delete" on the left side of screen, and click the atom ball you want to erase.

<mark>If you are going construct a new model:</mark>

c10. Pull down the bottom menu on the canvas, and select "build a new molecule".

c11. Input the name of the new molecule.

c12. Follow steps c3 - c6.

✓ *How can I **visualize** different models or molecules at the same time?*

v1. Construct molecules you want to view. If you have files of them, just go to menu bar "file" and "open" them.

v2. Select "visualize" button.

v3. Click "Views" and select 2 or 4 views.

v4. Pull down the left menu of each view and select molecule you want to view.

v5. Pull down the right menu on the bottom canvas, and select "wireframe" or "space fill." You can get other types of models.

✓ *How can I analyze chemical/physical properties based on molecular structures?*

a1. First, construct molecules you want to compare. If you have files of them, open those files.

a2. Click "Analyze" button. You can select "all molecules" to compare ("all molecules" here means those molecules being constructed or files being opened at that moment) or select "some molecules" to analyze only those molecules you want.

a3. Pull down the menu of properties, and choose "boiling point" or the property you want to compare. The values of properties are from a database, and we did not input all data of these properties yet. Hence you could only get some data like carbon count, atom count or boiling points of alkanes.

NOTE:

❑ Here is an easy way to attach all hydrogen atoms by one click. Select "extras" feature in the "construct" window. Click "fill in hydrogens."

❑ Remember to add ".alc" after the compound's name or you can't open the file next time.