WebAssign Java Molecular Editor (JME) Help

Written by Kay Sandberg

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How to Answer a JME Question

Click the "Open JME Editor" button.

Draw your answer in the JME Editor Window.

Click "Save Drawing".

Notice that a string of letters and characters are automatically entered in the WebAssign answer box. This string is called the SMILES string. It is an ASCII representation of the chemical compound.
If no JME window pops up, your browser may not be configured to allow use of Java. JME may not work on Macintosh computers.
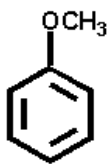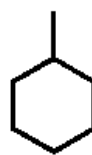
How JME Displays Carbons & Hydrogens

Carbons and hydrogens bonded to carbon are not shown explicitly when drawing skeletal structures in the JME editor.
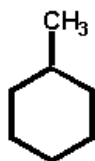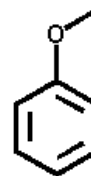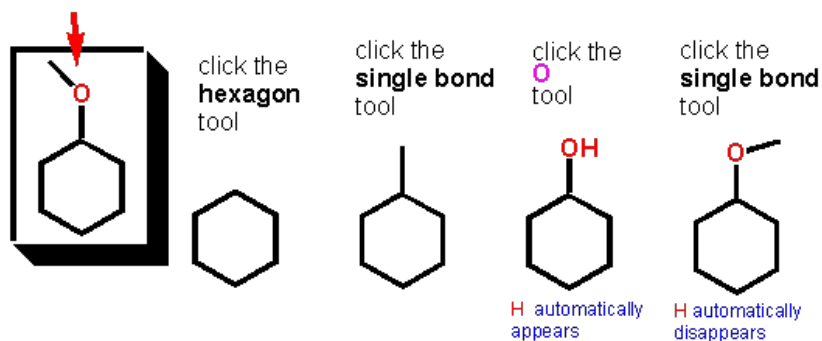
Examples

Hydrogens bonded to any other atom must be shown - the JME editor will automatically put them where needed.

Do not use the X tool to place hydrogens.

Hydrogens will automatically disappear when you click to make another single bond, a double, or a triple bond. Here is an example.

If this is what you want to draw, here is one way you can do it.

click the **hexagon** tool

click the **single bond** tool

click the O tool

click the **single bond** tool

H automatically appears

H automatically disappears

Do not use the X tool if an atom appears on the toolbar unless specifically instructed.

When to Use the X Tool

The X tool is located at the lower left of the JME.

Use the X tool when an element does not appear on the toolbar.

Use the X tool if instructed to do so in the question.

Do *not* use the X tool for an element that appears on the toolbar.

Do *not* use the X tool to add hydrogens to non-carbon atoms; hydrogens will be automatically added when needed for heteroatoms.

In skelatal structures:
(1) Carbon atoms are not shown explicitly - carbon atoms are understood to be at the end of bonds and at vertices.
(2) Hydrogens bonded to carbons are not shown in the skelatal structure - each carbon possessing a zero formal charge is understood to have as many hydrogens as needed to give the carbon access to an octet of electrons.

Realistic Bond Angles

Use realistic bond angles when drawing skeletal structures.

Entering unrealistic bond angles will result in a SMILES string which is different than the SMILES string for the correct answer.

Examples
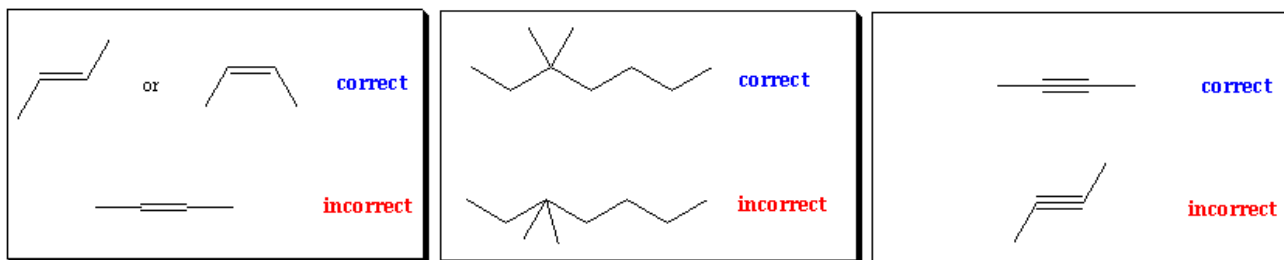
Cis-Double Bond Formation

Click the double bond tool on the toolbar.

Draw the double bond.

Click the single bond tool and add a single bond to one carbon of the double bond.

Still using the single bond tool, click on the other carbon of the double bond and with the mouse button held down, rotate the single bond around.

How to Use the Wedge/Dash Tool

When drawing skeletal structures where you need to show stereochemistry about tetrahedral carbons use the following formats.

(Please note: You should restrict your use of wedge/dash bonds to stereospecific reactions in which chiral carbons remain chiral or to indicate the stereochemistry on rings when stereospecific reactions are involved. If a carbon is not chiral and it is not part of a ring stereospecific site, you should not use wedge/dashed bonds.)

To make a wedge bond, use the wedge tool on the toolbar to click the atom where you want the wedge bond to appear.

To make a dash bond use the wedge tool on the tool bar to click the atom where you want the dash bond to appear. Make the wedge first and then click in the middle of the wedge bond to turn it into a dash bond.
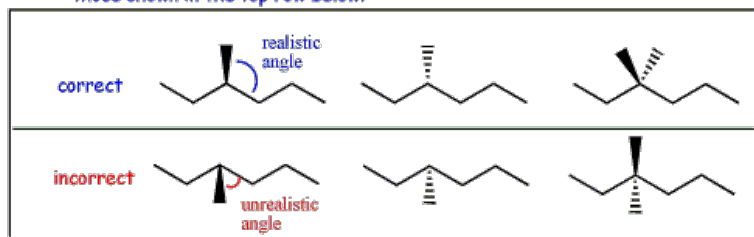
You can toggle back and forth between wedge and dash by clicking with the wedge tool in the middle of the bond.

Make sure the tapered end of the bond (the skinny end) is bonded to the parent or when a ring is involved, make sure the tapered end is bonded to the ring.

Examples
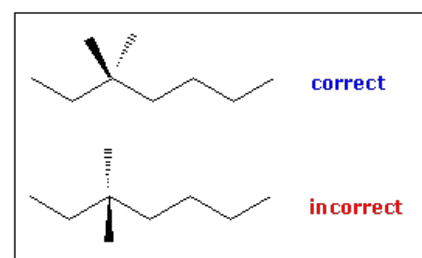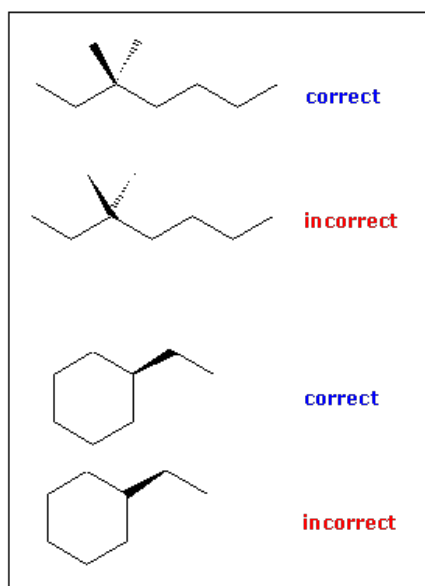
Make sure you use realistic angles when using wedge/dash bonds like those shown in the top row below.
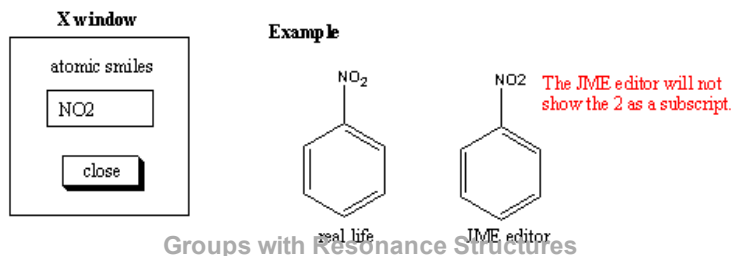

Nitro Group

When you need to add the nitro group, follow these steps.

Draw all of the bonds first. Do not draw the C-H bonds since they are understood.

Draw a single bond on the atom to which the NO_2 will be added.

Click on the X tool and type "NO2" in the X window.

Click on the end of the bond where you need the nitro group to appear.

Example

NO$_2$

NO2   The JME editor will not
show the 2 as a subscript.

real life   JME editor

Groups with Resonance Structures

When placing a group that has at least two resonance structures (such as the nitro group) on a benzene ring or alkyl parent you should not use bonds within the group, instead you should do the following.

Click the X tool on the tool bar.

Type in the formula for the group in the X window.

Click on the bond to which you want to attach the group.

Note: When using the X tool to type in formulas, the subscripts will appear as normal numbers (not subscripts). For example, if you needed to put an NO$_2$ as a branch, you would click the X tool, type in "NO2" and then click on the bond where you wanted the NO$_2$ to appear, but it would appear as NO2.

How to Show Formal Charge

When your structure contains an atom possessing a formal charge, follow these steps.

Draw a skeletal structure as if the charged atom did not possess a formal charge. Hydrogen atom(s) will appear as needed on non-carbon atoms to give the atom in question a zero formal charge.

Select the +/- tool from the top toolbar.

Click on the atom that should possess the formal charge. Click repeatedly until the formal charge you need appears. (You may have to click on the atom a couple of times until the correct formal charge appears.)

Hydrogen will be added or deleted with each click of the +/- tool as appropriate for the formal charge shown.

Grignard Reagents

Draw all of the bonds first. Do not to draw the C-H bonds, since they are understood and will not be shown.

Draw a single bond on the carbon to which the MgBr will be added.

Click on the X tool and type "MgBr" in the X window.

Click on the end of the bond where you need the MgBr to appear.

Example

X window

atomic smiles

MgBr

close

In order to show that the Mg is "sandwiched" between the C and X, you should orient molecule so that the MgBr is on the right side as shown below.

MgBr

Organolithium Reagents

Even though we conceptually think of an organolithium as possessing a carbon with a lone pair and negative charge for mechanism purposes, we include the bonded lithium in the organic product in synthesis schemes.

To input propyllithium in the JME editor:

First draw:

Open the X window (click the X tool on the toolbar).

Type "Li" in the X window.

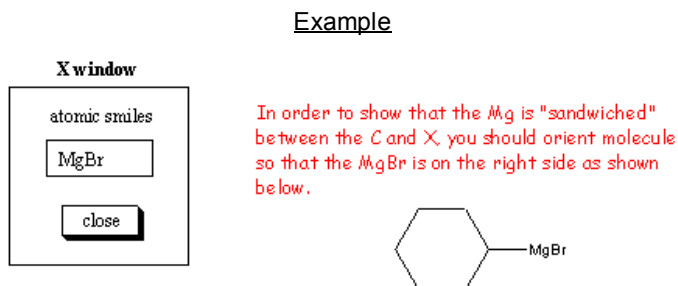Click on the end of the bond where Li needs to appear.

Deuterium Atoms

Draw all of the bonds first. Do not to draw the C-H bonds, since they are understood and will not be shown.
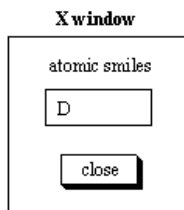
Draw a single bond on the atom to which the D will be added.

Click on the X tool and type "D" in the X window.

Click on the end of the bond where you need the D to appear.

Example

If C-1 of butane is deuterated by the reaction of butylmagnesium bromide with D_2O, then you would draw the following skeletal structure.

X window

atomic smiles

D

close

Example #1 If C-1 of butane is deuterated by the reaction of butylmagnesium bromide with D_2O, then you would draw the following skeletal structure.

Example #2 If a deuterated alcohol is needed:

1st draw

2nd click the O tool on the tool bar and add the O

Do **NOT** type **OD** in the X window box!!!!
Only type in the **D**.

3rd click the X tool and type D in the X window as shown in the diagram above and then click on the end of the bond.

When your product is a fused polycyclic system (two rings with adjacent carbon members of both rings), follow these steps.

Draw the first ring using one of the ring tools.

Select the appropriate ring tool for the second ring.

Click the bond of the first ring where you want the second ring to appear.

Cyclic Sugar

Groups angled up in the chair conformation or pointed up in the Haworth formula should be represented by wedges in the JME editor.

Groups angled down in the chair conformation or pointed down in the Haworth formula should be represented by dashes in the JME editor.

Hydrogens are understood.

Make sure the tapered end of the wedge or dash bond is attached to the ring.

To make a wedge bond use the "wedge" tool on the toolbar to click on the atom where you want the wedge bond to appear.

To make a dash bond use the "wedge" tool on the tool bar to click on the atom where you want the dash bond to appear. Make the wedge first and then click in the middle of the wedge bond to turn it into a dash bond. You can toggle back and forth between wedge and dash by clicking with the wedge tool in the middle of the bond.

Examples

Chair conformation

β-D-glucopyranose

Haworth formula

β-D-glucopyranose

JME editor input format
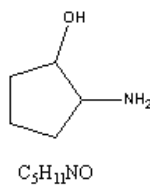
β-D-glucopyranose
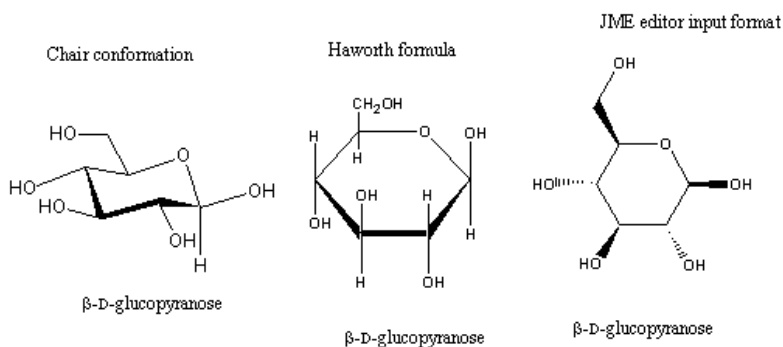
Molecular Formula Input

Follow the element order: CH and then alphabetically any other elements present.

A subscript of 1 is understood and should not be entered into the formula.

The following compound's molecular formula would be typed in as C5H11NO.

Example

$C_5H_{11}NO$

In the past there have been some students who have experienced weird problems with the editor (it is only a few out of hundreds). Here are some things to look out for:

1. After you have drawn your structure in the JME editor and click "save drawing," you should see a list of letters appear in the answer box of the question. This list of letters is called the SMILES string and it is the SMILES string with gets compared to the SMILES string in the answer key. **If the SMILES string does not appear and you submit, it will be counted incorrect.** Before you submit, make sure you have a SMILES string in each of the JME editor question answer boxes.
2. Some students have experienced disappearing SMILES strings on subsequent submissions. Here is the scenario: they will draw all of the structures and submit. They view the results and correct the structures that are missed. They submit again. All of the initially correct structures are gone and the answer box is missing the SMILES string - only the structures that were corrected have SMILES strings. This is a weird occurrence and only a few students have this happen. The WebAssign people cannot reproduce it and we can't figure out why this happens to only a few students. If you are one of the unlucky ones who experiences disappearing SMILES strings, there are two ways to combat this:
    I. On subsequent submissions open each JME editor of the ones which were graded correct, restore saved drawing, and then save drawing.
    II. Use a different browser or computer. If you are experiencing trouble with the JME editor using either Internet Explorer or Netscape, you may want to try Mozilla. Here is the website where you can go to download it: http://mozilla.org/
3. A structure may have several different SMILES strings, but **the important thing for you is to make sure you have the same SMILES string as the answer key** so you must heed the instructions given in the links of the question. **The biggest problem comes about if you use the X tool when not instructed to use it.** Elements added via the X tool have a different SMILES string than those added via the tool bar even though both of these SMILES strings produce the same structure. A student will compare his/her answer to the answer key and see that his/her structure is identical to the answer key's structure, but I'll look at the SMILES string and say, "Oops, you used the X tool, didn't you?!?!?!?!?" Since it is difficult to code the answer key with all of the possible SMILES strings when the X tool is used, I have restricted the use of the X tool to specific cases.

Bottom line: **please leave that X tool alone unless specifically instructed to use it or unless you need a non-hydrogen atom that does not appear on the tool bar.** Following this simple guideline will save you many minutes of frustration and several lost points.

JME X Window Troubleshooting

Procedure

First, CLOSE the JME Editor and the X-Tool window.

If you see a small icon in your system tray (the place where the time is displayed in the bottom right hand corner of your screen) which looks like a white coffee mug with red steam lines coming from it, right click on that and click "Open Console." A confusing window will pop-up. Press the letter "x" on your keyboard.

This will clear the class loader cache from your Java Applet plug-in, i.e., this clears whatever residual data/classes that were left behind from previous uses of the JAM editor.

If you do not see that nifty little icon in your system tray, visit the following link and click the "Update" button to download a package which will update your current browser with better JME capabilities (more or less).

http://java.sun.com/products/javawebstart/download.html

If you already have Java installed on your computer (and you almost certainly do) then you don't have to download the "Full" package, just the "Update."

After you've installed Web Start, you may or may not have this problem again. If and whenever you do, follow the "Procedure" given in the first part of this discussion post.