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Introduction

Lab Wizard is a ChemLab tool used to design chemistry lab simulations. Although ChemLab comes with a variety of lab modules, such as an acid-base titration, you need not limit your work to these pre-fabricated experiments. Lab Wizard will translate your labs into ChemLab modules called User Defined Lab (UDL's) by asking you to supply it with chemical data and reaction formulas. These UDL files can then in turn be traded and exchanged among your colleagues. Model Science Software will be glad to post your lab simulations for you at their web site.

Before you begin using the Lab Wizard, you should prepare the following:

(1) Introduction, Procedure, and Observations RTF files.

(2) a list of chemicals (reactants and products as well as all intermediate chemicals) along with any new data which you may need to add to the Chemical Database, and

(3) a draft of a list of reactions.

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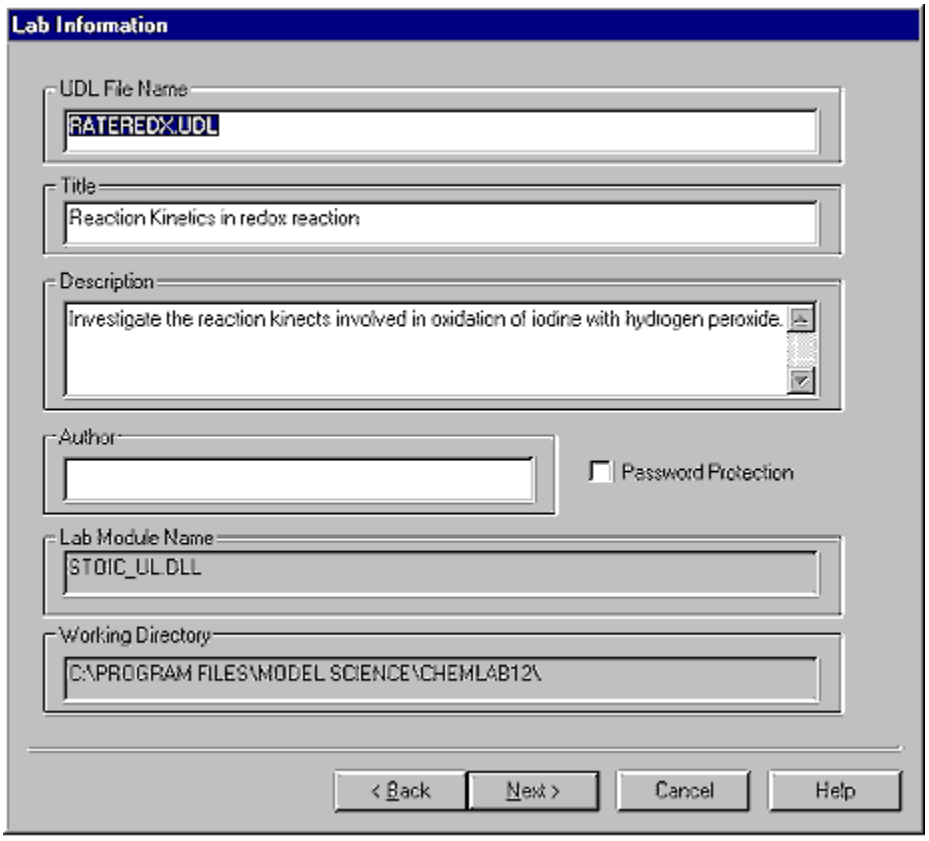
Information

Fill in the UDL File Name (you don't need to add the .UDL extension), lab Title and lab Description, then select Next.

This information will appear in the Simulation Module dialogue box.

Author is optional. (Note that you may include your e-mail address here.)

Password protection is available in order to prevent unwanted tampering with lab module design or viewing of information such as the names of unknown chemicals and other lab details.

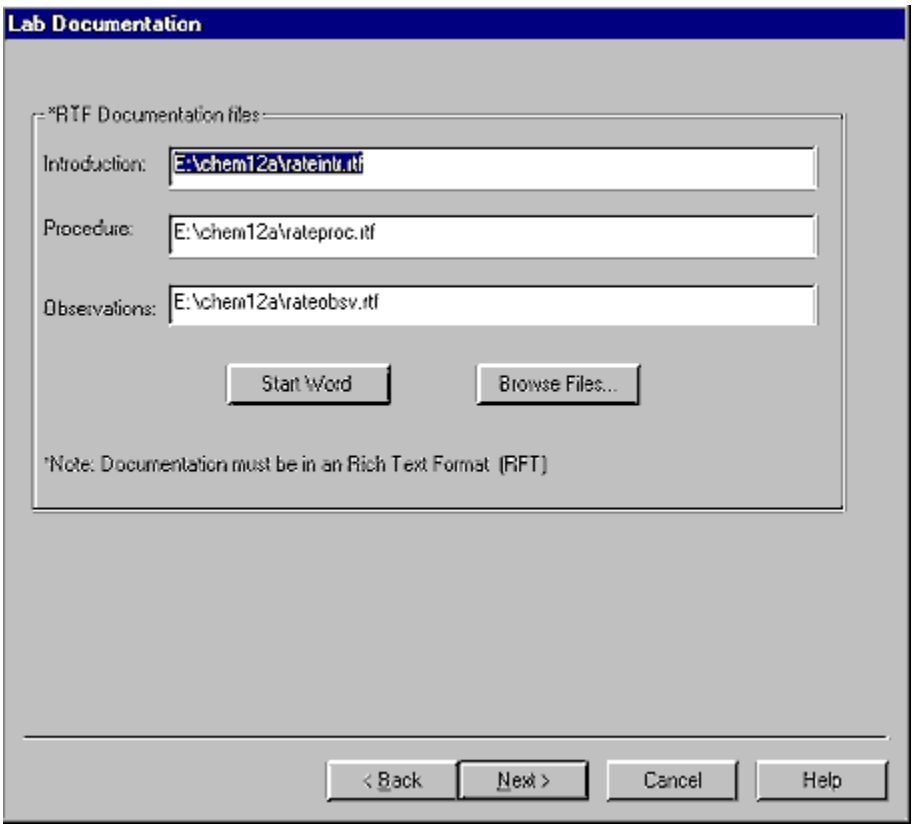


Documentation

Specify your Introduction, Procedure and Observations file locations (no need to provide extensions), then select Next.

If you haven't already created these documents, you may use any wordprocessor that can save in Rich Text Format (i.e.*.rtf). For your convenience, Microsoft Word maybe launched from this dialog box. If you highlight one of the fields and select Start Word, the file will be opened in Word. Once created, these files will be displayed in separate windows for your users on the left-hand side of Chemlab's environment . In the Introduction document you should include the reasons for conducting the experiment and the theory behind it, including the formulas for the reactions to be performed. In the Procedure document you should include the step-by-step instructions for conducting the experiment, making special note of the quantities of chemicals required. The Observation document should be formatted such that the items to be observed are listed on the left-hand side and blanks spaces are provided on the right-hand side. Users may then record observations and required calculations directly in ChemLab. Upon completion of the lab, users may save their results to a file, either on disk or on a network file server. If the lab is used as part of a student's course work, observations in the form of a lab file may be submitted for grading.

If you are editing a UDL provided to you without these files, the Lab Wizard will use the documentation information already stored in the UDL file.



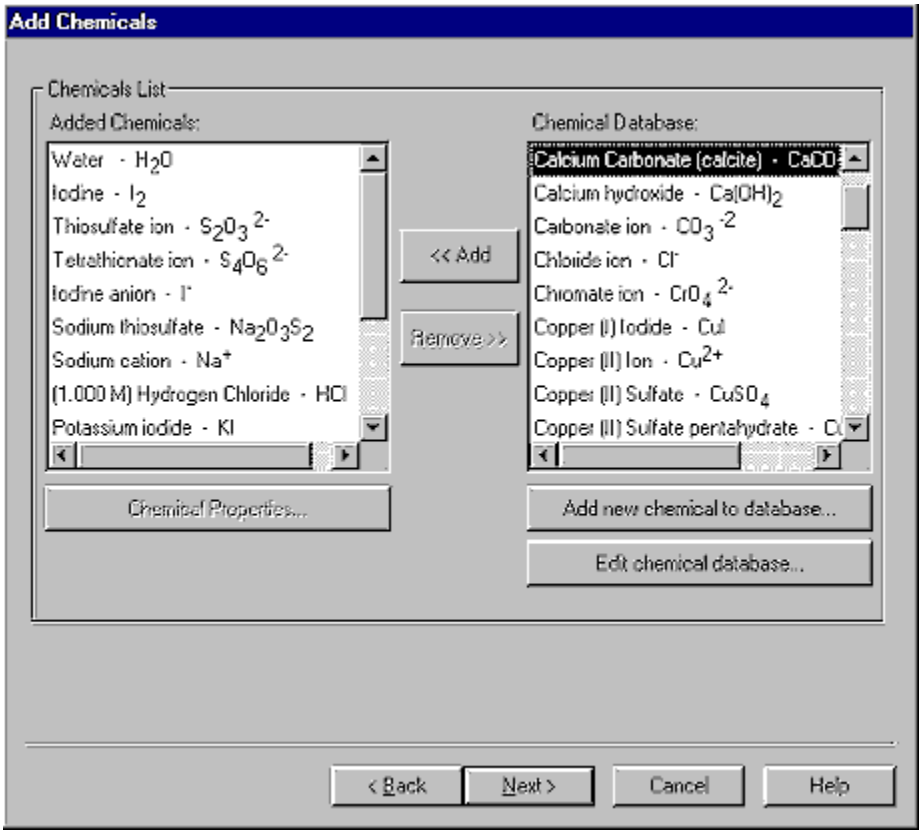
Chemicals

Before you create your customized lab module, you must check to make sure that all the chemicals required for your products, reactants, and all intermediate reactions used in the process are available in the Chemical Database. If they are not, don't panic. You can always add to the database yourself. (Note that water is automatically included in the Added Chemicals list.)

Use the Chemical Database scroll bar to search for each of the chemicals on your required chemicals list. If you find one, select << ADD and check it off your list. If you've added something you don't need in your lab, select Remove>> to delete it from the Added Chemicals list. Once a chemical has been imported from the database, its properties must be specified in the Chemical Properties dialog box. It appears automatically when a chemical is dropped, but may also be accessed by highlighting a chemical and selecting the Chemical Properties… button.

If new chemicals need to be added to the Chemical Database , select Add new chemicals to database ... .

If you need to change the specifications for a new chemical you've added to the database, you may highlight the chemical in the database column and select Edit chemical database ….



Reactions

The formulas for your chemical reactions are entered into the UDL by means of a reaction tree. Before using the Lab Wizard, you may want to draw a reaction tree for your experiment. The structure of the tree is the same as the familiar structure of file directories or folders found on a disk. The root directory is always Reactions. From here you must create separate sub-directories for each reaction, which in turn contain separate sub-directories for Reactants and Products.

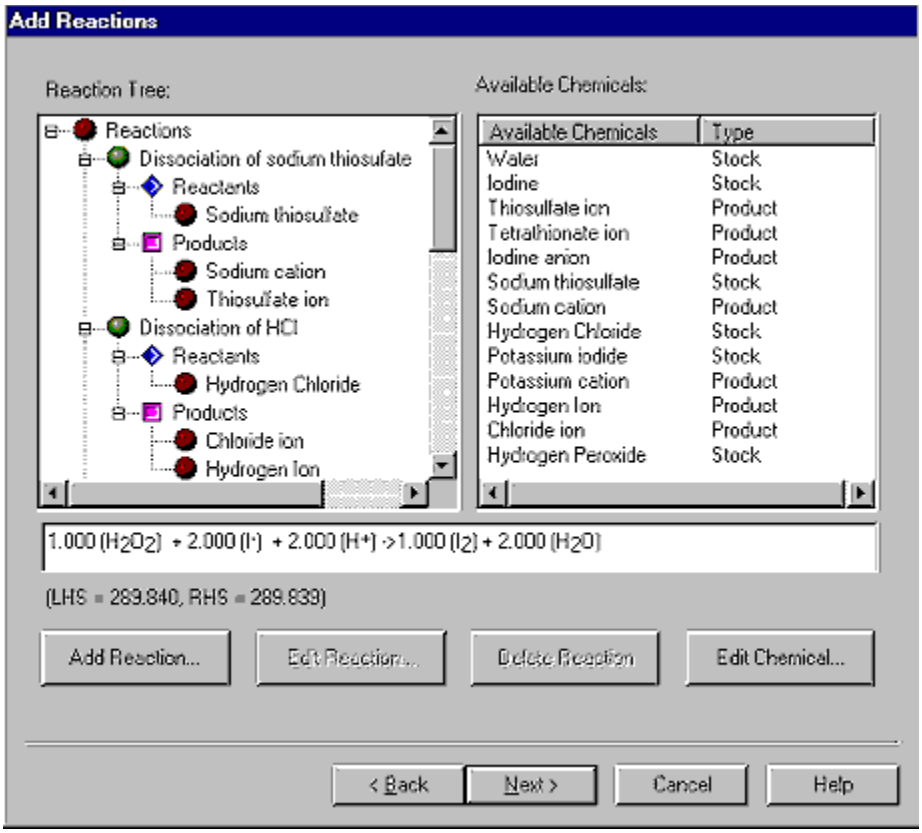
The order of reactions moving down the tree is the order in which reactions will be simulated by ChemLab's stoichiometry reaction engine. All dissociation reactions should be executed first. Some reactions will have precedence over other reactions. Hence, it's possible that one reaction may consume all the chemicals for another reaction before it begins, preventing it from occurring at all.

Start adding reactions by selecting the Add Reaction button. A Reaction Detail dialog box will appear. A new entry will appear in the Reaction Tree. Drag and drop chemicals from the available Chemical List to the leaf nodes labeled Reactants and Products. The "NO" symbol, the circle with the slash through it, indicates where chemicals may not be dropped.

Once reaction tree nodes are in place reactions may easily be manipulated by highlighting a particular reaction node and clicking on the right mouse button. A context menu appears which offers four options: Edit Reaction…, Delete Reaction, Move Up, or Move Down.

Once chemicals have been dropped they may easily be edited or deleted by highlighting a particular reactant or product and clicking on the right mouse button.

Clicking on a reaction node displays the chemical formula for the reaction along with the mass balance for the left-hand side (LHS) and the right-hand side (RHS) of the equation. Looking to see whether or not the LHS and RHS values are equal is a quick way to check that the formula was entered correctly.


Add Reactions
Reaction Tree:
Reactions
Dissociation of sodium thiosulfate
Reactants
Sodium thiosulfate
Products
Sodium cation
Thiosulfate ion
Dissociation of HCl
Reactants
Hydrogen Chloride
Products
Chloride ion
Hydrogen Ion
Available Chemicals:
Available Chemicals
Type
Water Stock
Iodine Stock
Thiosulfate ion Product
Tetrathionate ion Product
Iodine anion Product
Sodium thiosulfate Stock
Sodium cation Product
Hydrogen Chloride Stock
Potassium Iodide Stock
Potassium cation Product
Hydrogen Ion Product
Chloride ion Product
Hydrogen Peroxide Stock
1.000 (H2O2) + 2.000 (I-) + 2.000 (H+) ->1.000 (I2) + 2.000 (H2O)
(LHS = 289.840, RHS = 289.839)
Add Reaction...
Edit Reaction...
Delete Reaction
Edit Chemical...
< Back
Next >
Cancel
Help

Chemical Database

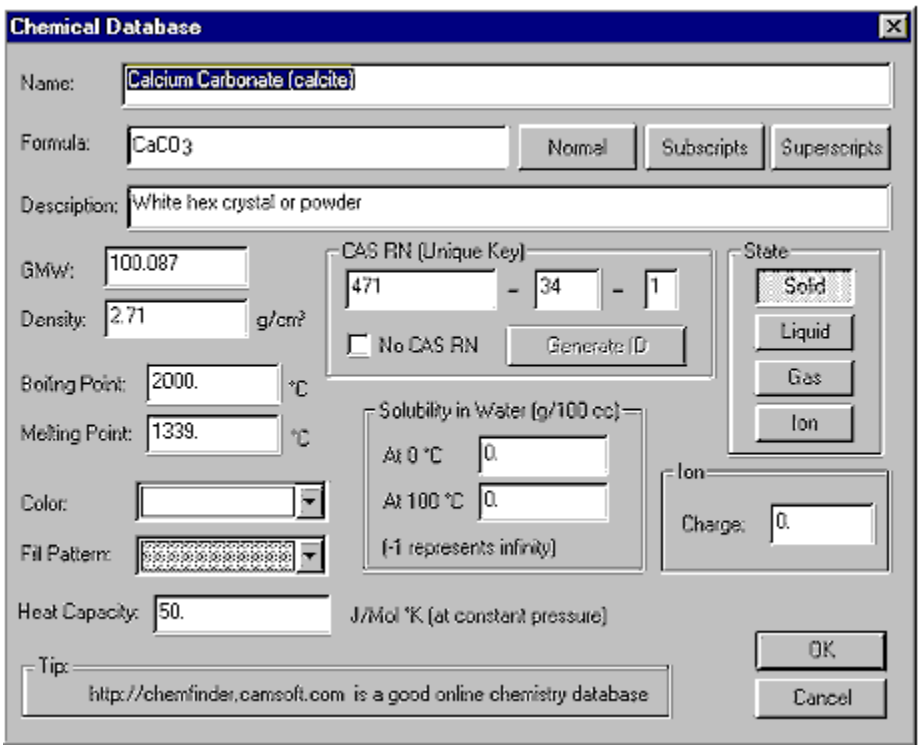
Here is a form that must be filled out for each new chemical that is added. You will probably need to do some research. Chemlab uses solubility to determine how much of a substance is in solution. Ions are produced by the dissociation of a compound in solution. For example, HCl becomes H+ and Cl- in solution. If ions are required for intermediate reactions, then they must be added to your chemical list from the database.

The following web sites may be helpful for chemical research:
http://www.cas.org
http://chemfinder.camsoft.com
http://www.krinfo.ch/krinfo/products/datastar/sheets/CSEM.HTM
http://www.chem.ucla.edu/chempointers.html
http://www.dojindo.co.jp/products/info/castest.html

The following are the properties listed for each new chemical in ChemLab's Chemical Database:

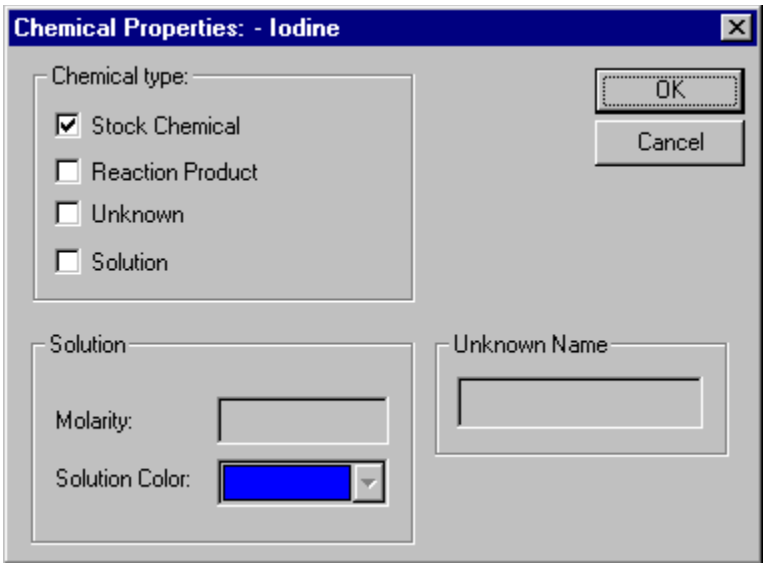
Name:	
Formula:	
Description:	
GMW:	(required for all chemicals)
Density:	g/cm3 (optional for ions)
Boiling Point:	oC (optional for ions)
Melting Point:	oC (optional for ions)
Color:	(see color dialog box)
Fill Pattern:	(used to indicate crystal, powder, or sold)
Heat Capacity:	J/Mol oK (at constant pressure)
Ion Charge:	(e.g. –1 or +2)
State:	(Solid, Liquid, Gas, or Ion)
Solubility in Water	
at 0 oC :	
at 100 oC :	
CAS RN: _____ - ___ - __	(CAS registry number)

Hint: Copy this form and Paste it into a word processor document so you can print multiple copies for research purposes.


Chemical Database
Name:
Calcium Carbonate (calcite)
Formula:
CaCO3
Normal
Subscripts
Superscripts
Description:
White hex crystal or powder
GMW:
100.087
Density:
2.71
g/cm³
CAS RN (Unique Key)
471
-
34
-
1
No CAS RN
Generate ID
State
Solid
Liquid
Gas
Ion
Boiling Point:
2000.
°C
Melting Point:
1339.
°C
Solubility in Water (g/100 cc)
At 0 °C
0.
At 100 °C
0.
(-1 represents infinity)
Ion
Charge:
0.
Color:
Fil Pattern:
Heat Capacity:
50.
J/Mol °K (at constant pressure)
Tip:
http://chemfinder.camsoft.com is a good online chemistry database
OK
Cancel

Chemical Properties

The Chemical Properties dialog box appears after a chemical is dropped into the reaction tree. Of particular importance is classifying each chemical as either a Stock Chemical, a Reaction Product, a Unknown, or a Solution. Some of these properties are exclusive. A Reaction Product cannot also be a Solution. Solutions are prepared according to the specified molarity (e.g. 1 M HCl) and, along with Stock Chemicals, are provided to the ChemLab user in the available chemicals list in the Chemicals dialog box. Since Reaction Products are produced by a reaction, they are not available to the user and do not appear in the chemicals list. An Unknown chemical is a reactant to be solved for by the user. The name specified under Unknown Name appears in the available chemical list in place of the chemical's actual name.



Reaction Details

Name reaction and set any reaction conditions.

Reaction Rates maybe set as instantaneous, fixed, or varying with concentration.
Instantaneous is self-explanatory. Fixed rate means that the reaction occurs at the rate the first reactant is consumed in mole/L(sec). Setting this rate simulates a reaction occurring over a period of time. For a reaction that varies with concentration, the rate of reaction may set to depend upon the concentration of reactants. Given the reaction:

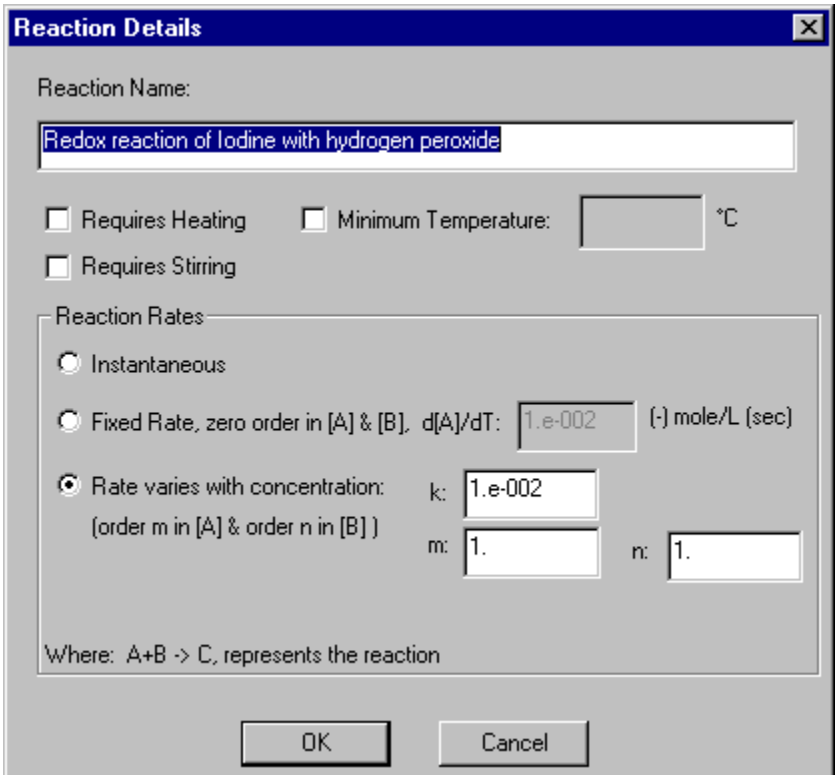
A + B -> C

The reaction rate is expressed as the rate of change of the concentration of the first reactant. The relationship that exists may be expressed as:

rate = d[A]/dt = k([A]^m[B]^n)
or rate of change of the concentration of X

where K = rate constant, (units are M/s)
m = order of the reaction with respects to the concentration of A
n = order of the reaction with respects to the concentration of B

ChemLab only allows for the rate to be affected by the concentration of the first two reactants only. The positioning of chemicals when adding a reaction is therefore important.



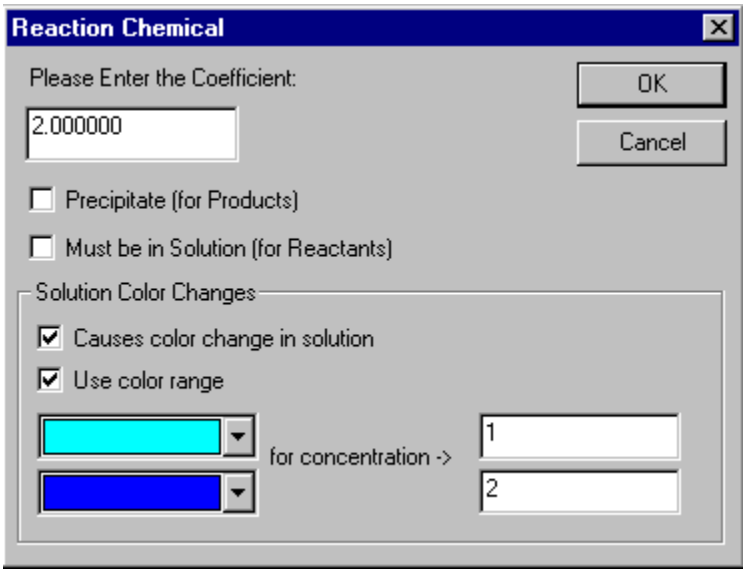
Reaction Chemical

The Reaction Chemical dialog box appears when you drag a chemical from the Available Chemicals list and drop it as a reactant or product. It is used to enter the coefficient for the chemical and assign attributes that affect the appearance and use of the chemical in the reaction.

(1)The "Precipitate" check box indicates that a product is shown as a solid precipitate when formed.

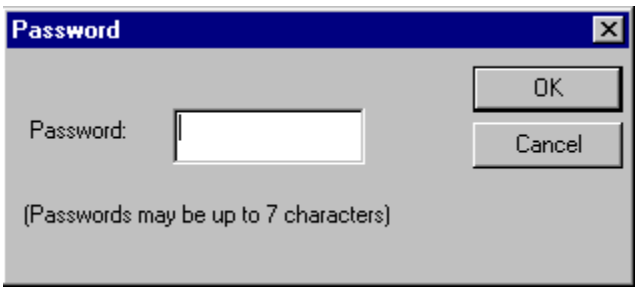
(2)The "Must be in solution" check box indicates that a reactant which is a solid must be dissolved into a solution before it is used in the reaction. This is typical of dissociation reactions of the form AX(aq) -> A- + X+.

(3) The "Solution Color Changes" option is used to cause a change in the color of a solution to indicate that this chemical has been produced. The change option is set by selecting the Causes color change in solution" check box. The color of the solution will change instantaneously to whatever color has been selected on the left-hand side when the chemical reaches the molar concentration entered on the right-hand side. If you wish the color change to be gradual, you must select the "Use color range" checkbox. The color of the solution will change gradually over the range of colors specified on the left-hand side as the concentration of the chemical increases or decreases as specified on the right-hand side. Note that only one color change will be shown by ChemLab. Hence, you should only mark one product in a reaction to change solution color. If a number of reactions are set to cause a color change, only the color change for the last active reaction will appear.



Password

Password usage is optional. It's a good idea if you want to prevent your students hacking into the lab module. However, if you plan to distribute this UDL, you will have to send the password along with it. Otherwise, it will be useless to others. Note that you can remove password protection by deselecting the check and re-entering the password.



Finish

Select Finish and the new UDL will be generated by the Lab Wizard and placed in the ChemLab directory.

Close and restart ChemLab. Select your newly created lab from the ChemLab Simulation modules dialog box.

Remember that making a UDL is an iterative process. You will probably have to run through several trials before you get your new lab working properly.

Web Site

The Model Science Software web site is: http://www.modelscience.com .

This is where you may post your UDL's for other ChemLab users and download from our UDL library as it builds with contributions made by users like you.

You may launch your web browser by selecting Model Science Web Page from the ChemLab Help Menu.

User Defined Lab

A User Defined Lab (UDL) is a single, distributable file that contains the information included in the RTF files for introduction, procedure, and observations as well the chemicals and reactions specified in the lab. Hence, the UDL is complete. There is no need to include any other files when distributing a UDL to another ChemLab user.

Using Microsoft Word

If you launch Microsoft Word to edit or create any files, remember that these files must be closed in Word before you return to the Lab Wizard to generate your UDL file. If the files aren't closed, the Lab Wizard will not have permission to read them. Note that this feature does not support other types of word processors.

CAS Registry Number

The chemicals in the ChemLab database are indexed according to their Chemical Abstracts Service Registry Number. Therefore, they must be unique. If you can't find a number for a particular chemical, the Lab Wizard will generate one for you. However, this should only be done as a last resort. See http://www.cas.org .