

MODEL SCIENCE SOFTWARE INC.

MODEL CHEMLAB LAB WIZARD TUTORIAL

SIMULATIONS FOR THE CLASSROOM, LAB
AND INTERNET

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Lab Wizard Introduction

The Lab Wizard is a tool used to design chemistry lab simulations for use with Model ChemLab. It is bundled with the Model ChemLab Professional Edition for instructors.

The Lab Wizard steps the user through the process of creating a lab simulation. The user enters the lab details, including documentation text, chemicals, indicators, lab reactions and other data. The user can go back and forth through the Lab Wizard screens, making many changes until the final lab is complete and working correctly.

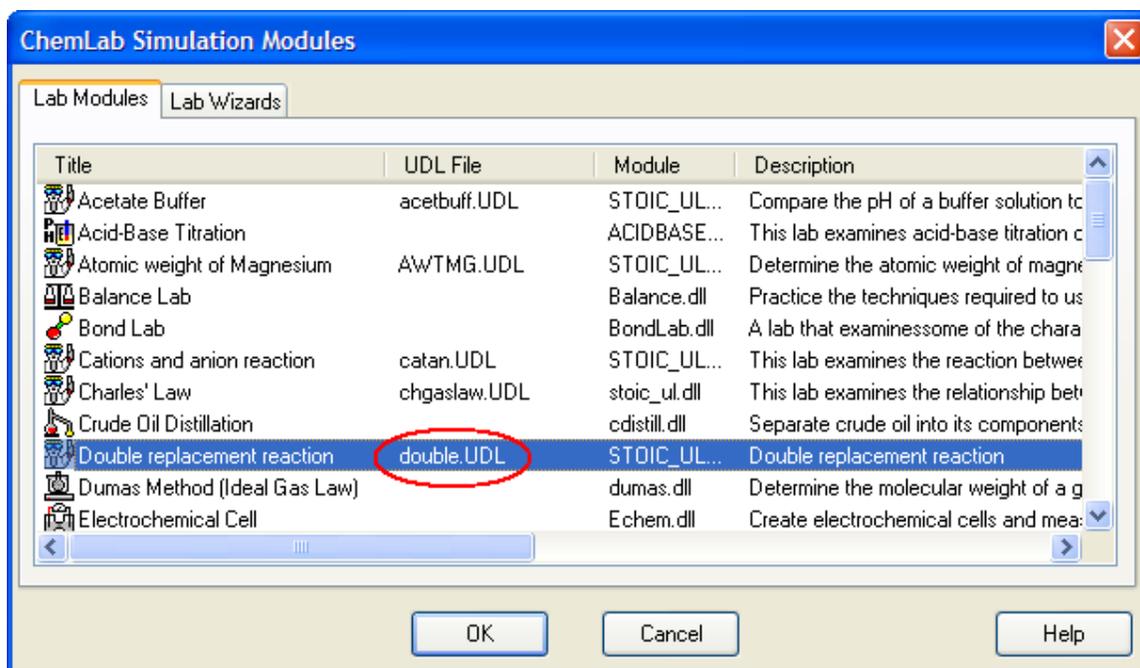
The Lab Wizard takes these details and creates a “UDL” file that contains data and instructions. The file can then be loaded by students using the Standard Edition of the software or edited by users using the Professional Edition of the software.

These UDL files will be listed in the ChemLab Simulation Modules dialog box, which appears at start-up or when a New lab is selected from the File menu.

With ChemLab there are two types of simulations files: 1) those that are created using the Lab Wizard tool (.udl files) and 2) those that are pre-programmed extensions to ChemLab (.dll files). Note: The Windows long extension for “.UDL” is “.UDL-CHEMLAB”.

If a simulation was created using the Lab Wizard it will have an entry in the “UDL file” column.

For example, the *Double replacement reaction* was created using the Lab Wizard and has an entry in the UDL File column labelled *double.udl*.

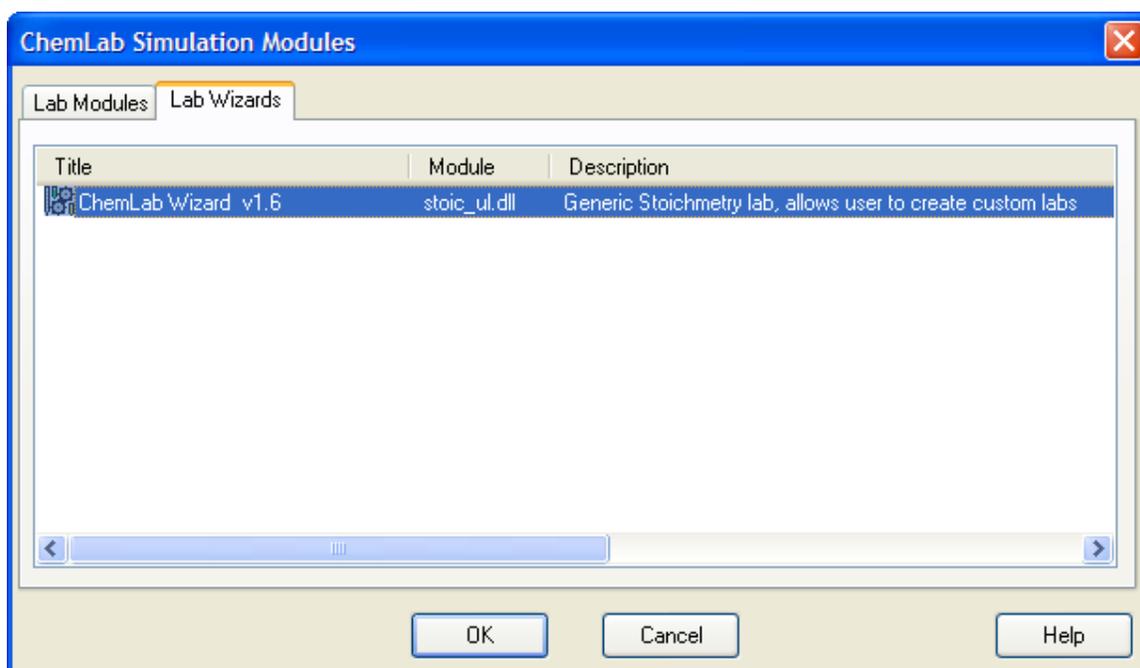


Starting the Lab Wizard

Step 1: Start ChemLab or select New lab from the File menu.

Step 2: Select the Lab Wizards tab from the ChemLab Simulation Modules dialog box.

Step 3: Select the ChemLab Wizard and press the OK button.



Preparing to use the Lab Wizard

Before using the Lab Wizard, you should be able to answer the following questions:

What chemicals are involved?

Will you be using unknown chemicals?

What type of reactions (displacement, addition, substitution, redox, acid-base, etc.)?

Will the reactions occur instantaneous or over time?

Will you be using indicators?

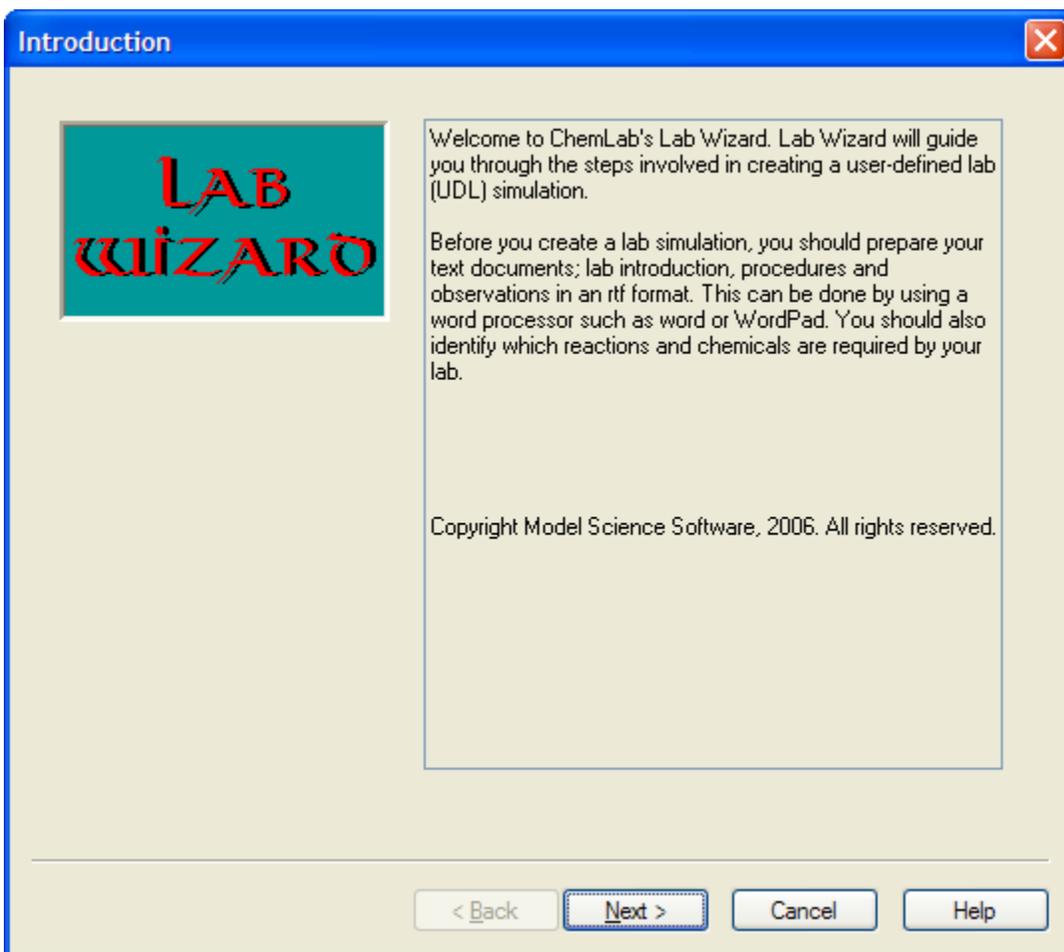
Will there be any color changes?

What is the lab procedure?

What is the lab introduction?

What observations should be collected?

Lab Wizard Introduction Screen



This is the welcoming screen to the Lab Wizard. There are no data inputs. You just select next and move onto the next screen.

Context sensitive Help (F1): If you press the Help button or F1 key you will receive the context sensitive Help for that dialog box or screen.

“Next” and “Back” Buttons: Like other program wizards, the ChemLab LabWizard allows the user to step forward and backwards through a series of screens until the lab simulation is ready and working correctly. The “Next” and “Back” buttons are used to navigate between the various screens of the Lab Wizard.

Lab Information Screen

This screen is where the general information about the simulation is entered.

The screenshot shows a 'Lab Information' dialog box with the following fields and values:

- UDL File Name:** C:\Program Files\Model Science\ChemLab Pro\HexaneBromination.UDL
- Title:** Light-Catalyzed Bromination of Hexane
- Description:** Light-Catalyzed Bromination of Hexane
- Author:** (empty)
- Lab Module Name:** stoic_ul.dll
- Working Directory:** C:\Program Files\Model Science\ChemLab Pro\
- Password Protection:**

Navigation buttons at the bottom: < Back, Next >, Cancel, Help.

1. UDL File Name Field: This field is the file name for the simulation. If no extension is added to the file name, the program will add the “.udl or .udl-chemlab” extension. It is not necessary to include a path. The path will always be the same as the ChemLab working directory and is added by the program.
2. Title: This field is the lab title that is displayed in the ChemLab Simulation Modules dialog box under the “Title” column.
3. Description: This field is an optional short description of the simulation. It is displayed in the “Description” column of the Simulation Module dialog box.
4. Author Name: This optional field is for the name of the author.
5. Password protection: Selecting this field restricts access to the subsequent screens to only those users who know the password.

Lab Documentation Screen

In this screen the user identifies the lab documentation that will be included with the lab simulation. The text in these files will appear in ChemLab in the Text Window panes when the simulation is loaded.

These files must be in RTF (Rich Text File) format. RTF files can be created using Microsoft Word or other word processor programs. Both the Introduction and Procedures will appear as read-only in ChemLab, which means the student cannot edit them. However, the Observations text can be edited by the student, allowing observations to be saved in a .lab file and sent to the instructor for evaluation.

Lab Documentation

*RTF Documentation files

1 Introduction: ogram Files\Model Science\ChemLab Pro\UDL Docs\HexaneBromideIntro.rtf

2 Procedure: ogram Files\Model Science\ChemLab Pro\UDL Docs\HexaneBromideProc.rtf

3 Observations: iles\Model Science\ChemLab Pro\UDL Docs\HexaneBromideObservation.rtf

4 Start Word Browse Files...

*Note: Documentation must be in an rich text format (RFT)

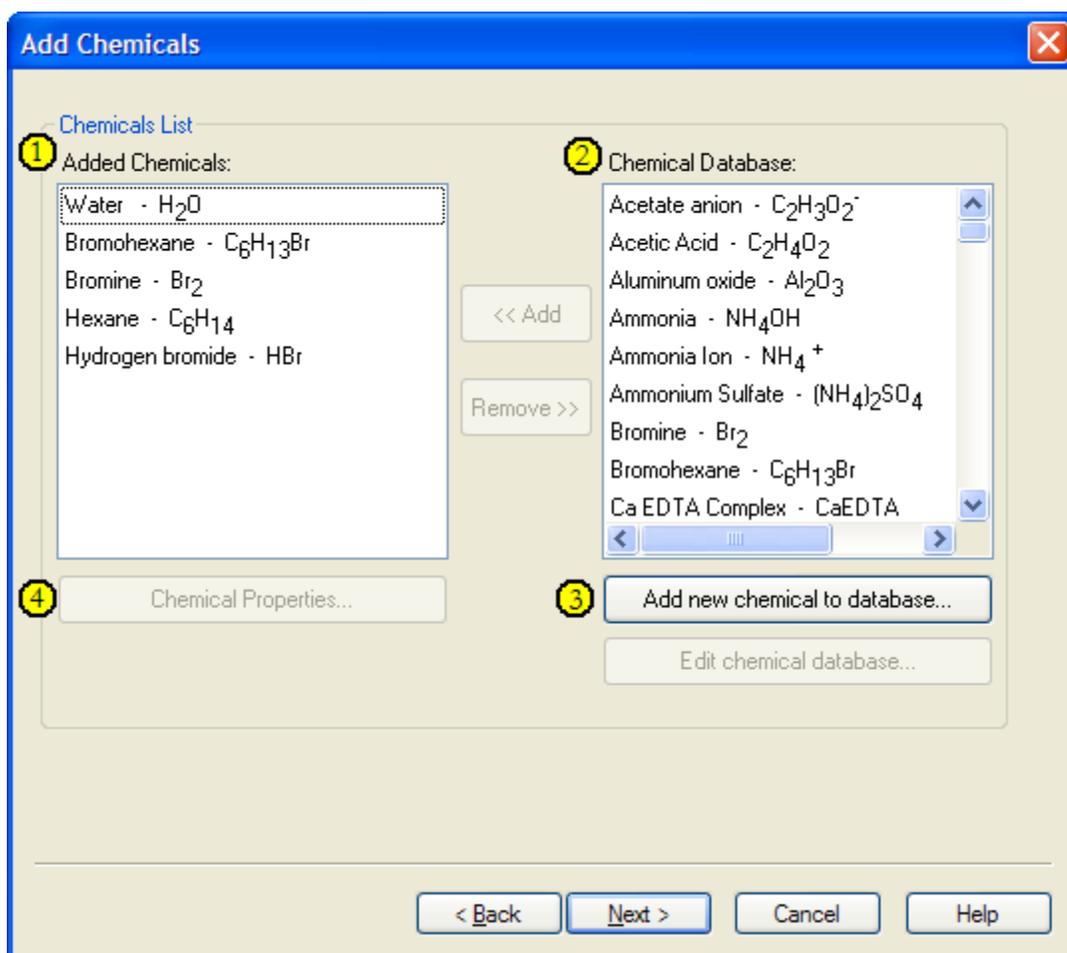
< Back Next > Cancel Help

1. Introduction: This is the theory or lab introduction that is displayed in the Lab Introduction pane of ChemLab. To add an introduction file to the simulation, select the Introduction field and press the “Browse Files...” button. This will open a file dialog box. Using the File dialog locate the RTF (Rich Text Format) file you would like to use for the Introduction text.

2. Procedure: This is the set of instructions that the student will perform in the lab. You add the Procedure file the same way that you added the Introduction file.
3. Observations: This is the text that the student will fill in during the lab. The observations that the student makes can be saved in the ChemLab .lab file. You add the Observations file the same way that you added the Introduction file.
4. Starting Word: If you select one of the text document fields and press the “Start Word” button that file will be opened in whatever word processor is associated with the .rtf file type. The default is usually Microsoft Word.

Add Chemicals Screen

In the Add Chemicals screen the user adds all the chemicals that will be used in simulations, including all reactant and products.



1. Added Chemicals: This is the list of chemicals that will be included in the lab simulation.

2. Chemical Database: This is a file containing all chemicals that can be added. The user selects the chemical to be added from the Chemical database list and presses the “Add” button. This will add the chemical to the Added Chemicals list.
3. Add new chemical to database: If a needed chemical is missing from the database it can be added using the “Add new chemical to database” button. Once added the chemical will be available for use in future lab simulations. (See Chemical Database).
4. Chemical Properties: When a chemical is added to the list of chemicals a dialog box opens that requires the user to detail its properties once in the Added Chemical list. These properties can be also be edited by selecting a chemical in the Added Chemical list and pressing the “Chemical Properties...” button.

Chemicals Properties Dialog

The chemicals properties dialog box will appear whenever a chemical is added to the list of chemicals or when a chemical is selected and the “Chemical Properties...” button is pressed.

Chemical Properties: - Sodium Chloride

Chemical type:

- 1 Stock Chemical
- 2 Reaction Product
- 3 Unknown
- 4 Solution

OK
Cancel

Solution

5 Molarity: 0.0

6 Solution Color: [dropdown]

7 Unknown Name: [input field]

Flame Test

8 Flame Test Color: [dropdown]

Conductivity Curve (Solutions)

9 Conductor: Coefficient A: [input field]
Coefficient B: [input field]

Prime Solution Settings

Where: $\text{Conductivity} = A \cdot \text{Molarity} - B \cdot \sqrt{\text{Molarity}}$

Chemical Types:

1. Stock Chemicals: In ChemLab a stock chemical is any chemical that the student is required to add to a container. These chemicals will appear in the “All Chemicals” dialog box in the main ChemLab program. Water is always included and is always a stock chemical.
2. Reaction Product: In ChemLab a reaction product is a chemical that is the product of a reaction. These chemicals can later act as reactants in other reactions.
3. Unknowns: These are usually stock chemicals whose identity you wish the student to determine. When a chemical is marked as an unknown the “Unknown Name” field will become writeable. The name typed in the unknown name field is the name the chemical will be labelled when the student runs the simulation.
4. Solutions: This is a solution of a chemical with water as the solvent. When this option is selected the Molarity and the Solution Color fields will become writeable. The user must enter a Molarity for the solution. For example: 1M NaOH solution is NaOH with a solution option and 1.0 entered for the Molarity field.

8. Flame Test:

The Flame test option allows user to perform flame test when a chemical is placed on a metal wire and burned in a Bunsen burner. The user first selects the flame test check box and selects a color from the color drop down control.

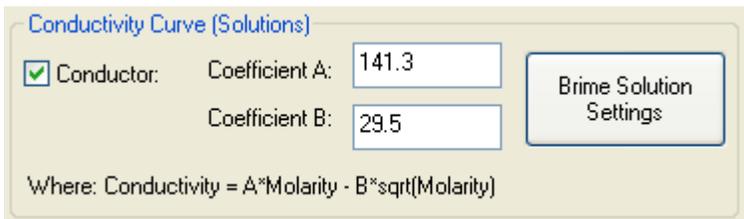


Note: The flame test will also require that the metal wire option is select in the Lab option Screen.

9. Conductor:

The conductor option allows a user to include conductivity data for a chemical solution. This data can then be used by a conductivity meter to calculate the electrical conductivity for a chemical in solution. Conductivity is calculated based on the following equation:

$$\text{Conductivity} = A * (\text{molarity}) - B * \sqrt{\text{molarity}}$$



To include conductivity data the Conductor checkbox must be checked and values for the A & B coefficients values must be entered.

By selecting the “Brine (Salt) Solution Settings” button; default values will be entered for the A and B coefficient values.

Note: You must also select the conductivity meter equipment option in the Lab Options screens; to be able to test for a electrical conductivity in a chemical solution.

Chemical Database Dialog

The chemical database is a flat file in ChemLab called “chemicals.cdb” and is located in the working directory of ChemLab.

The chemical database dialog is used to add and edit entries in the chemical database. These entries are added to the UDL files chemicals list.

The dialog box can only be opened from the “Add Chemical” screen, using the “Add new chemical to database...” button or the “Edit chemical database...” button.

The screenshot shows the "Chemical Database" dialog box with the following fields and values:

- Name: Hexane
- Formula: C₆H₁₄
- Description: colorless liquid
- GMW: 86.18
- Density: 0.6548 g/cm³
- Boiling Point: 69. °C
- Melting Point: -95. °C
- Color: (empty dropdown)
- Fill Pattern: solid
- Heat Capacity: 50. J/Mol °K (at constant pressure)
- CAS RN (Unique Key): 110 - 54 - 3
- State: Solid (selected)
- Solubility in Water (g/100 cc): At 0 °C: 0., At 100 °C: 0.
- Ion Charge: 0.

Numbered callouts (1-12) are placed over various input fields in the dialog.

1. Name: This is the name of chemical.
2. Formula: This is the chemical formula. You can enter subscripts and superscripts to the formula by pressing the “Superscripts” or “Subscripts” button.
3. Description: This is a short description of the chemical.
4. GMW: This is the gram molecular weight of the chemical or what 1 mole of the chemical weighs.
5. Density: This is the chemical density.
6. CAS RN: This is Chemical Abstract Services Registry Number. This is a unique number assigned by the American Chemical Society used to identify chemicals. If you do not have a CAS RN number; you can create a unique identifier using the “No CAS RN” check box and pressing the “Generate ID” button. However, if you use this option it will be problem for other users to edit your UDL files unless they also have a copy of your “chemical.cdb” file.
7. State: This is the state of the chemical, usually solid, gas or liquid. If a chemical is listed as an ion then its density, boiling and melting point fields will be ignored.
8. Boiling and Melting points: These are the boiling and melting points for the chemical. If a chemical does not have a value for these because it decomposes, mark the appropriate “no melting point” or “no boiling point” checkboxes.
9. Solubility in Water: These values are used to determine the solubility of a chemical in water at a given temperature. ChemLab will extrapolate between the cold and warm water temperatures to arrive at the correct solubility. Usually a chemical is more soluble at a warmer temperature of water. If you do not know the exact solubility value, then enter a value of 100 for soluble substance or >10 for a slightly soluble substance. If a chemical is insoluble in water, enter a value of 0. If a chemical is infinitely soluble enter a value of -1.
10. Color and Fill Pattern: You can select a color and fill pattern for a chemical from the drop down combo lists. If a color is missing from the list, select the “other...” option and a colors dialog box will open. The fill pattern is not used for liquids, gases, ions or solutions of a given chemical.
11. Heat Capacity: This value is currently only used when a calorimeter is included. If you do not know the value, enter a value of 50.
12. Ion Charge: Is a value that is not used by the Lab Wizard engine. It may be used in the future. Only enter a value if you have an ion with a known charge.

Data for the chemical database entry can be found in CRC handbook of chemistry and physics or online at a number of free Web site, for example:

at <http://chemfinder.com> chemicals can be searched by formula or names,

at <http://en.wikipedia.org/> chemicals can be searched by formula or names,

at <http://google.com> search for chemical databases with data on a particular chemical.

Add Reactions Screen

The Add Reactions Screen enables the user to define the list of reactions that ChemLab will try to solve using numerical methods.

1 Reaction Tree:

- Reactions
 - Hexane Bromination Reaction
 - Reactants
 - Hexane
 - Bromine
 - Products
 - Bromo-hexane
 - Hydrogen bromide

2 Available Chemicals:

| Available Chemicals | Type |
|---------------------|---------|
| Water | Stock |
| Bromohexane | Product |
| Bromine | Stock |
| Hexane | Stock |
| Hydrogen bromide | Product |

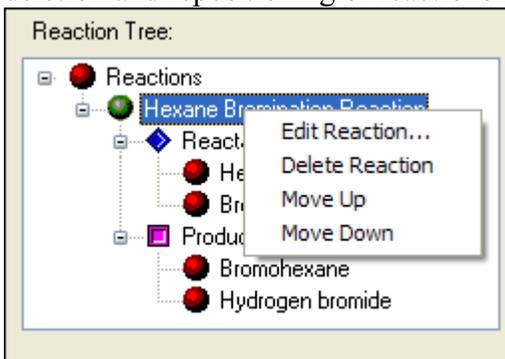
1.000 (C₆H₁₄) + 1.000 (Br₂) -> 1.000 (C₆H₁₃Br) + 1.000 (HBr)
(LHS = 245.990, RHS = 245.985)

3 Add Reaction... Edit Reaction... Delete Reaction Edit Chemical...

< Back Next > Cancel Help

1. Reaction Tree: List of the reactions that will be performed in the order that you want ChemLab to solve them. Reactions higher in the tree can prevent lower reactions from occurring by consuming all their reactants.
2. Available Chemicals: List of all the chemicals available to construct reactions. If a chemical is not present, you will need to go back to the previous screen and add it to the list of chemicals. Chemicals from the “Available chemicals” list can be dragged and dropped onto either the Reactants or Products branches of a reaction.
3. Add Reaction button: The first step in creating a reaction is to add a new reaction to the reaction tree. A reaction consists of all the reactant and products as well as conditions and settings for that reaction.

The Reaction Tree has (right-mouse click) context sensitive menus that allow editing, deletion and repositioning of reactions in the tree.



Reaction Details Dialog:

The 'Reaction Details' dialog box contains the following fields and options:

- 1** Reaction Name: Hexane Bromination Reaction
- 2** Requires Heating
- 3** Requires Stirring
- 4** Requires Light
- 5** Minimum Temperature: [] °C
- 6** Maximum Temperature: [] °C
- 7** Use Heat of Reactions: [] KJ
- 8** Use chemical equilibrium: []
- Reaction Rates**
 - 9** Instantaneous
 - 10** Fixed Rate, zero order in [A] & [B], $d[A]/dT$: 8.e-002 (-) mole/L (sec)
 - 11** Rate varies with concentration:
 - k: 8.e-002
 - (order m in [A] & order n in [B])
 - m: 0.
 - n: 0.

Where: $A+B \rightarrow C$, represents the reaction

Buttons: OK, Cancel

The reaction details dialog box is opened when a new reaction is added to the reaction tree or when an existing reaction's properties are edited.

The reaction details include the required reaction conditions and settings for the reaction rate, heat of reaction and equilibrium constant.

1. Reaction Name: Is the name that will appear in the Reaction Tree.
2. Requires Heating: Is a condition that requires the reaction to be heated by an external heating source. The heat source can be a Bunsen burner, hot plate or a hot water bath. If no heat source is provided, the reaction will not occur.
3. Requires Stirring: Is a condition that requires stirring of the contents. The stirring can be from the stirring rod or magnetic stirrer. If no stirring is applied, the reaction does not occur.
4. Requires Light: Is a condition that requires that an external light source be applied for the reaction to occur. If no external light source is applied the reaction does not occur.
5. Minimum Temperature setting: Is the minimum temperature that is required for a reaction to occur. Check the checkbox for minimum temperature and add a value to the minimum temperature field. If the minimum temperature is not reached or exceeded, the reaction will not occur.
6. Maximum Temperature Setting: Is the maximum temperature that is allowed for a reaction to occur. Check the checkbox for maximum temperature and add a value to the maximum temperature field. If the maximum temperature is exceeded, the reaction will not occur.
7. Use Heat of Reactions: Is the setting to use heat of reaction with a reaction. A reaction may be exothermic or endothermic. To set a value for the heat of reaction check the checkbox for "Use heat of reaction" and add a value to the heat of reaction field.

For example in the Heat of Neutralization Lab, the neutralization reaction is:
 $\text{HCl} + \text{NaOH} \rightarrow \text{NaCl} + \text{H}_2\text{O} + \text{heat}$; where heat = -55kJ

| | | |
|--|-----------------------------------|----|
| <input checked="" type="checkbox"/> Use Heat of Reactions: | <input type="text" value="-55."/> | KJ |
|--|-----------------------------------|----|

8. Use chemical equilibrium: Is a setting for the equilibrium constant for a reaction. To set this value, check the check box for equilibrium constant and add a value to the equilibrium constant field.

For example, with the dissociation of water, the equilibrium constant = 1×10^{-14}
 $\text{H}_2\text{O} \rightleftharpoons \text{H}^+ + \text{OH}^-$

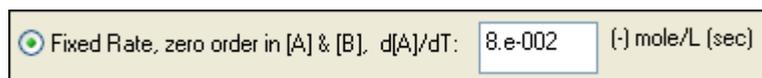
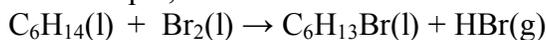
| | |
|---|--------------------------------------|
| <input checked="" type="checkbox"/> Use chemical equilibrium: | <input type="text" value="1.e-014"/> |
|---|--------------------------------------|

9. Instantaneous: Is one of three possible settings for the rate of a reaction. Reactions that have a setting value of instantaneous will occur immediately. This is the default value for a reaction.
10. Fixed Rate, zero order: Is a reaction that will occur over time independent of the concentration of the reactants. This value is often used to create a reaction that does not happen instantly but over a short period of time. The rate constant refers to the rate of change of the concentration of a reactant.

Where for the reaction $A + B \rightarrow C$, $\text{rate} = d[A]/dt$

In ChemLab the rate always refers to the first reactant in the reaction. All other reactants will be consumed based upon the stoichiometric ratio to the first reactant.

For example, for the reaction:



In this experiment, 25ml of Hexane (.189 moles) are mixed 2ml of Bromine (.039 moles). Since the stoichiometric ratio of Hexane to Bromine is 1:1, bromine is the limiting factor. Therefore .039 moles of Hexane will be consumed in this reaction.

Rate constant = Change Concentration of Hexane / time

Time = Change concentration of Hexane /Rate constant

$$\text{Time} = (.039/.027)/.08 = 18 \text{ sec.}$$

Therefore, this reaction will take 18secs to complete.

11. Rate Varies with concentration (or first order reaction): In this type of reaction the rate of reaction varies with the concentration of the reactants.

For example, in the lab “Reaction Kinetics of a Redox Reaction” there is the reaction of hydrogen peroxide with iodine whose rate is dependent upon the concentration of H_2O_2 and I^- :



The reaction rate is expressed as the rate of change of concentration of the participating species. In this case, the reaction rate, in terms of change of hydrogen peroxide concentration, may be expressed as:

$$\text{Rate} = d[H_2O_2]/dt = k[H_2O_2]^m[I^-]^n$$

where K = rate constant, (units are M/s),
 m = order of the reaction with respect to the concentration of hydrogen peroxide,
 n = order of the reaction with respect to the concentration of iodine ion,

It is given that, in this reaction, rate is independent of the concentration of H^+ .

| | |
|---|---|
| <input checked="" type="radio"/> Rate varies with concentration: (order m in [A] & order n in [B]) | k: <input type="text" value="1.e-002"/> |
| | m: <input type="text" value="1."/> n: <input type="text" value="1."/> |

ChemLab can handle the case of a 1st order reaction with up to 2 reactants. These must be the first and the second reactants.

Reaction Chemical Dialog:

When a chemical is added to a reaction the Reaction Chemical dialog box will appear. This dialog box enables the user to specify the coefficient of the chemical in the reaction and other settings that trigger color change or the appearance of a precipitate.

The screenshot shows the 'Reaction Chemical' dialog box with the following elements:

- 1. A text input field containing '1.000000'.
- 2. A checkbox labeled 'Precipitate (for Products)' which is unchecked.
- 3. A checkbox labeled 'In Solution' which is unchecked.
- 4. A checkbox labeled 'Gas from Atmosphere' which is unchecked.
- 5. A checked checkbox labeled 'Causes color change in solution'.
- 6. A checked checkbox labeled 'Use color range'.
- 7. A checked checkbox labeled 'Always perform color test'.
- 8. A dropdown menu showing a white color swatch, with '(low)' to its right.
- 9. A dropdown menu showing a red color swatch, with '(high)' to its right.
- Two text input fields for concentration: the first contains '5.e-002' and the second contains '0.1'.
- Buttons for 'OK' and 'Cancel'.

1. Enter the Coefficient: This is the coefficient of the chemical in the reaction formula.
2. Precipitate(for Products): This option allows a solid product to appear as a precipitate that will settle over time.
3. In Solution: Choose this option if the reactant or product is required to be in solution for the reaction to occur.
4. Gas from Atmosphere: This option allows an atmospheric gas such as oxygen to be used as a reactant. When this option is chosen it assumed that an unlimited supply of gas is present from the atmosphere for the reaction.

5. Causes color change in solution: This option allows a chemical to cause a change in the appearance of the liquid layer in a container. Choosing this option will enable the low concentration color drop box and concentration field.

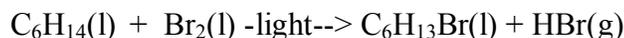
For example:

Causes color change in solution Always perform color test
 Use color range
 (low) 1.0
 for concentration ->
 (high)

This set of options will cause a solution color change when the chemical reaches a minimum concentration of 1 molar in the container.

6. Use color range: This allows a graduated color change to occur over a range of concentrations. When this option is checked both the high and low concentration color drop downs and edit fields will be enabled.

For example, in the experiment “Light-Catalyzed Bromination of Hexane”, there is a color change from brownish red to transparent when the reactant bromine (Br_2) is consumed by the reaction and concentration falls below .05 molar.



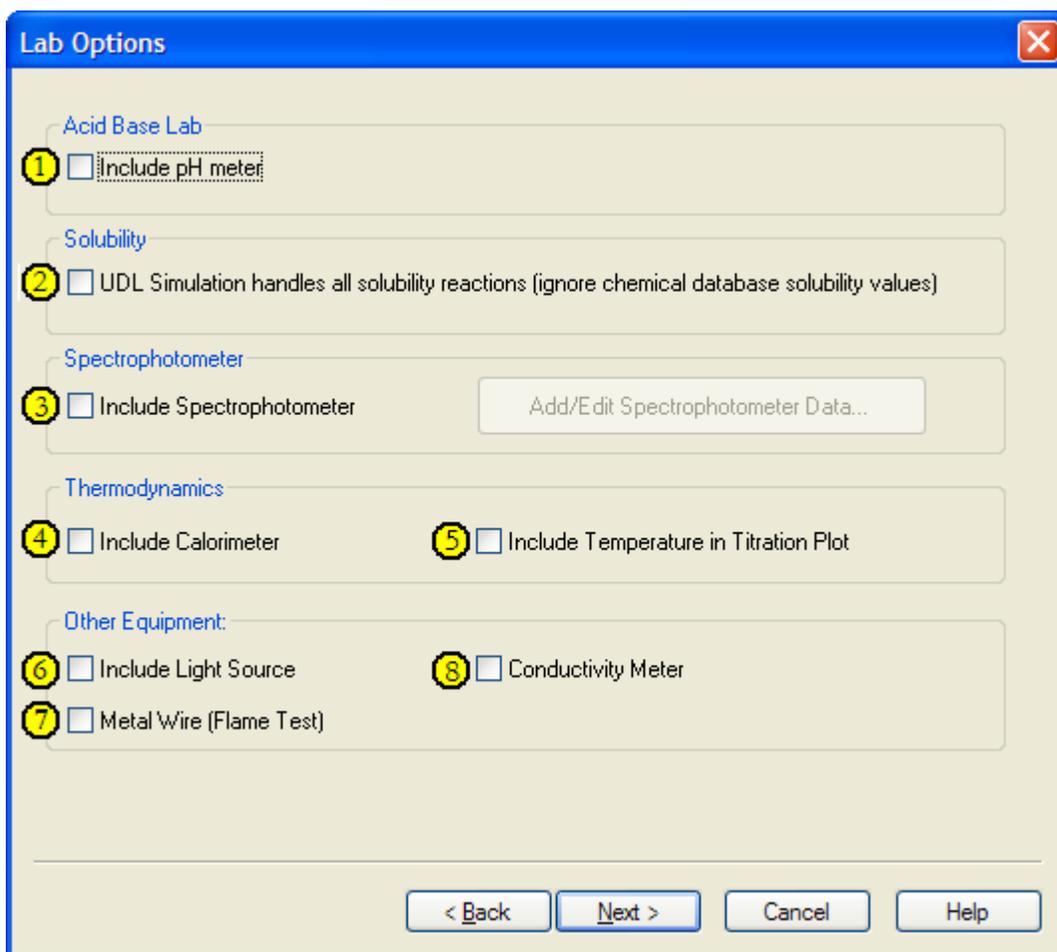
Causes color change in solution Always perform color test
 Use color range
 (low) 5.e-002
 for concentration ->
 (high) 0.1

Note: in ChemLab white represents transparency since the background color is white.

7. Always perform color test: This is an option that causes the simulation to test for a color changing chemical, even if the reaction doesn't occur or the chemical is completely consumed by a reaction.

Lab Options Screen

The Lab Option screen enables the setting of a number of different options for a lab simulation, such as adding additional lab equipment or changing the default solubility behaviour of ChemLab.



1. **Include pH meter:** This option is used when creating an acid-base lab simulation. Setting this option will enable selection of a pH meter from ChemLab's Equipment menu. Only use this option if you have set up the necessary reactions for an acid-base lab. This will also activate the titration plot menu options for the lab, enabling the plotting of a pH curve.
2. **UDL Simulation handles all solubility reactions:** This option turns off the default solubility behavior in ChemLab. The default behavior is based on the cold and hot water solubility entries in the Chemical Database. By disabling the behaviour, these entries will be ignored and ChemLab's default solubility behavior will not be active. Instead, solubility will be handled by the reactions included in the simulation. If you set this option, you may need to include your own solubility equilibrium reactions to handle solubility.

3. Include Spectrophotometer: This option will enable selection of a spectrophotometer from ChemLab's Equipment menu. In creating a lab simulation that includes a spectrophotometer you must add data points for the molar extinction coefficient (shown as k). Pressing the "Add/Edit Spectrophotometer Data..." button will open the Spectrophotometer Data dialog box.

Spectrophotometer Data Dialog:

| Chemical | Wavelength | K value |
|-----------------------------|------------|------------|
| Cobalt Chloride hexahydrate | 510 nm | 500.000000 |
| Cobalt Chloride hexahydrate | 400 nm | 200.000000 |
| Cobalt Chloride hexahydrate | 300 nm | 100.000000 |
| Cobalt Chloride hexahydrate | 600 nm | 50.000000 |

Add/Modify Data Points

Chemical: Cobalt Chloride hexahydrate

Wavelength (nm):

K Value:

Add New Data Point

Update Data Point

Remove Data Point

OK Cancel

The Spectrophotometer Data dialog enables the Lab Wizard user to add, edit and delete data points for a particular chemical in solution at a given wavelength.

New Data is added by entering the Chemical, Wavelength and K value and then selecting the "Add New Data Point" button.

The "Chemical" drop down will list all the available chemicals in the simulation. First select the chemical, then enter values for wavelength and k value for that wavelength. Pressing "Add New Data Point" will enter the new data in the "Current Data Points" list.

An existing data point can be edited by selecting the data in the “Current Data Point” list, changing the chemical, wavelength or k value, and then selecting the “Update Data Point” button.

A data point can be deleted by selecting the data in the “Current Data Point” and then selecting the “Delete Data Point” button.

Note that it is assumed that the solvent is water. It is also assumed that the path length is 1 cm for the spectrophotometer arrangement in ChemLab.

If you include more than one data point for a given chemical over a range of wavelengths, ChemLab will interpolate k-values between the data points.

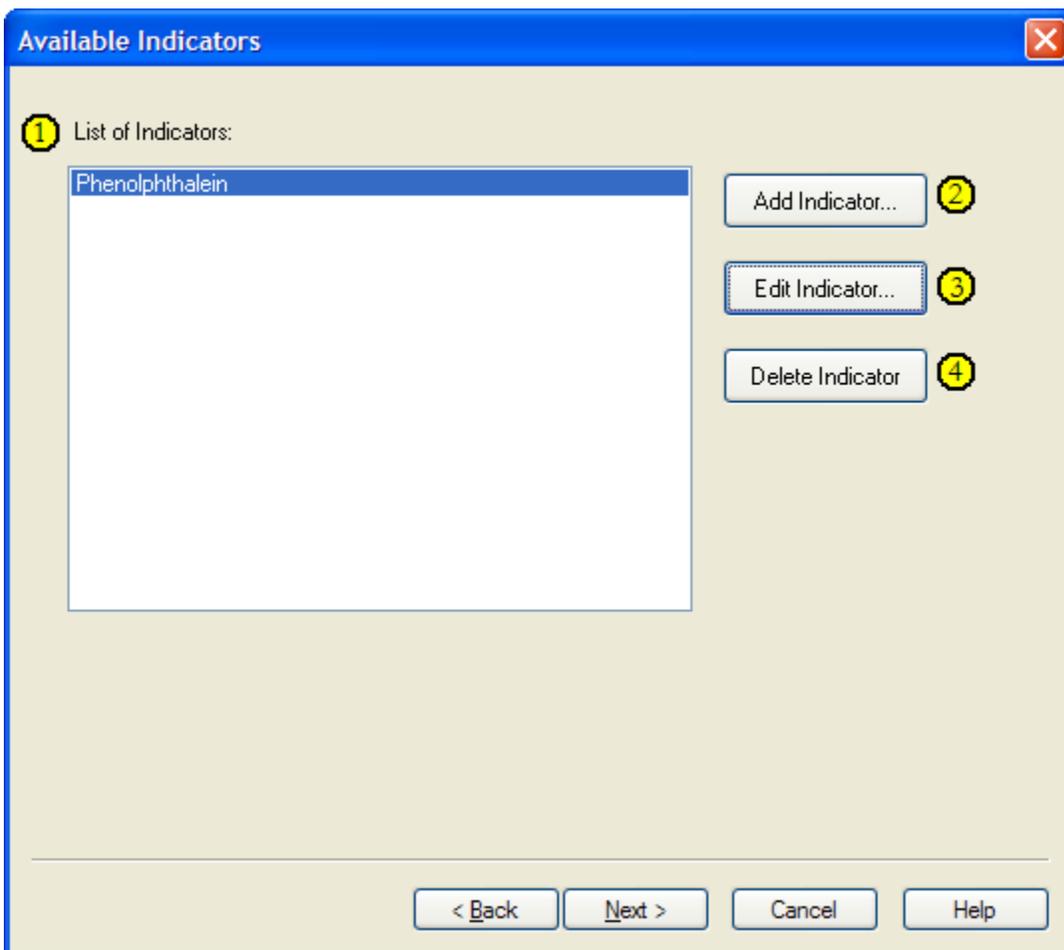
4. Include Calorimeter: This option will enable the selection of a calorimeter in the Equipment menu for this simulation. The calorimeter is an insulated container that prevents its contents from cooling or warming to the surrounding room temperature. This option is used in conjunction with the specific heat settings from the chemical database to create labs like the specific heat lab.
5. Include Temperature in Titration Plot: For acid-base labs that include a pH-meter, this option will include the temperature with the titration curve. Only include this option if you have also included heat of neutralization for your reaction.
6. Include A Light Source: This option will make a light source available in the equipment menu. This is used with the reaction condition requiring a light source for reaction to occur.
7. Metal Wire (Flame Test): This option will make a Metal wire for use in a flame test lab available in the equipment menu. This is used in conjunction with the Chemical properties dialog for a chemical's flame color.
8. Conductivity Meter: This option will make a conductivity meter available in the equipment list so that a chemical solutions electrical conductivity can be tested. This is used in conjunction with settings for chemical conductivity in the Chemical properties dialog.

Available Indicators Screen

This Lab Wizard Screen enables the user to add indicators to the lab simulation. Indicators in ChemLab are accessible through the “Indicators...” menu. The Available Indicators dialog box lists the indicators that maybe selected.

Indicators are used to signal the presence of a chemical in a certain concentration by causing a color change.

Indicators are treated differently from other chemicals in ChemLab. For example, they do not need to have an entry in the chemicals database. Instead, they are accessed using the indicators dialog box. Only one indicator may be used at a time in a container and they do not take part in reactions. Finally, they have no mass or volume in ChemLab.



The Available Indicators screen lists all the indicators added to a simulation and allows the user to add, edit or delete indicators from the simulation.

1. List of Indicators: Is a list of all the indicators currently included in the simulation. Selecting an existing indicator will enable the Edit Indicator and Delete Indicator buttons.
2. Add Indicator: To add a new indicator press the “Add Indicator...” button. This will open the Indicator Properties dialog box.
3. Edit Indicator: To edit an existing indicator, select the indicator from the list of indicators and press the “Edit Indicator...” button. This will open the Indicator Properties dialog box with the settings for that indicator.
4. Delete Indicator: To delete an existing indicator, select the indicator from the list of indicators and press the “Delete Indicator...” button.

Indicator Properties Dialog:

The Indicator Properties dialog box allows the user to define the details and behavior for the indicator.

Indicator Properties

Indicator Name: Phenolphthalein

Indicator Description: Changes from colorless to pink as pH goes from 8 to 10

Indicates presence of chemical: Hydroxide Ion In solution

Measures pH

Color Change:

(low) 8.

for concentration/ pH -> 10.

(high)

Caused initial color change in solution:

OK Cancel

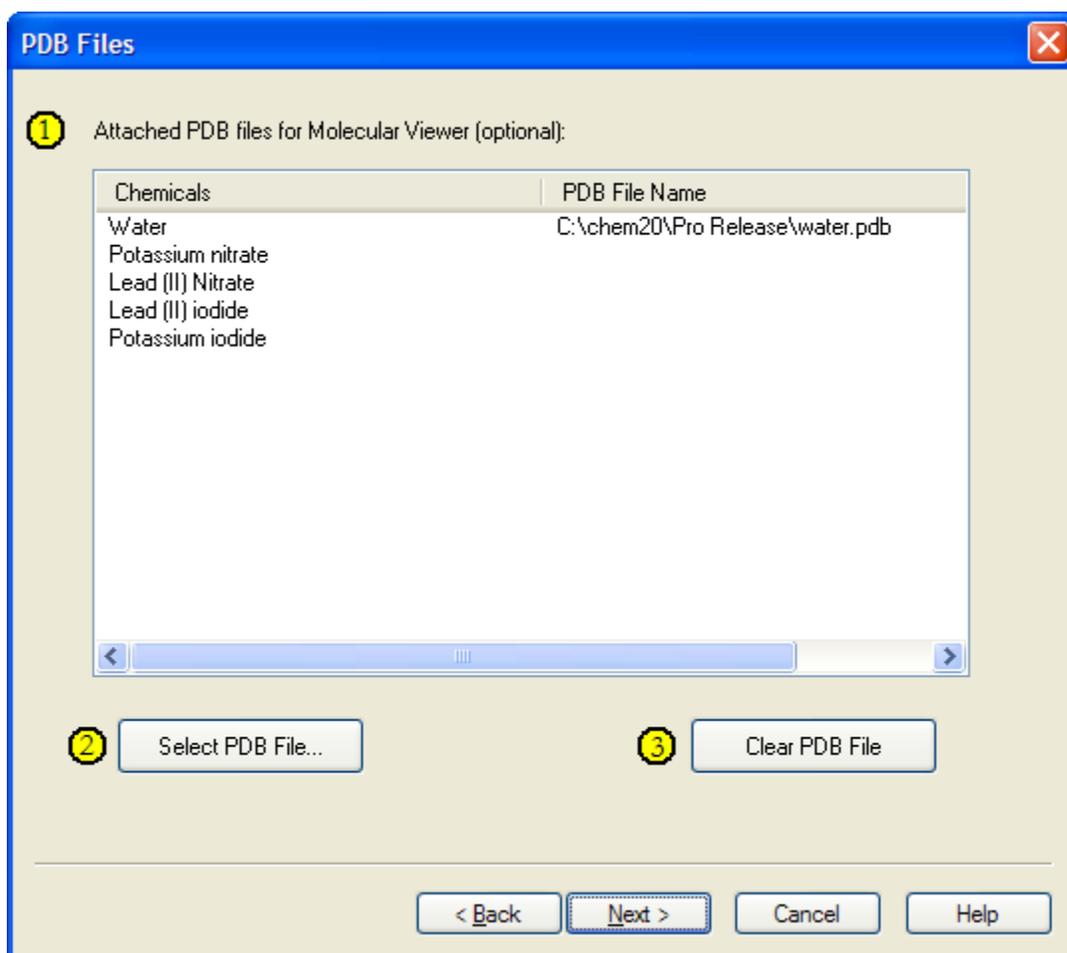
1. Indicator Name: Is the name that will appear in the Lab Wizard's List of Indicators and in ChemLab's Indicators dialog box.
2. Indicator Description: Is a short description of the indicator that appears in ChemLab's Indicators dialog box. This is usually used to describe what color change is caused by the indicator.
3. Indicated presence of chemical: An indicator can be used to indicate the presence of a chemical. The Chemicals drop down list will display all the available chemicals in the lab. If the chemical must be in solution, then also check the "In Solution" checkbox option.
4. Measures pH: If the indicator is used to measure pH, then check this option. This will also disable the chemicals drop down list and "In Solution" checkbox.

Note: pH values can only be used for an indicator when the Acid Base Lab Include pH meter option is set.

5. Color Change: The color change drop down list allows the user to define the color change that will occur. The user can also define a range of color changes over a range of concentration or pH values.
6. Caused initial color change in solution: This checkbox and color drop down list can be used if the addition of the indicator causes an initial color change in the solution in the absence of the chemical the indicator is testing for.

PDB Files Screen

The PDB (Protein Database) Files screen enables the user the option to attach a PDB file to a chemical. The PDB files can then be viewed using the RasMol molecular viewer program from the Chemicals Properties dialog box within the ChemLab.

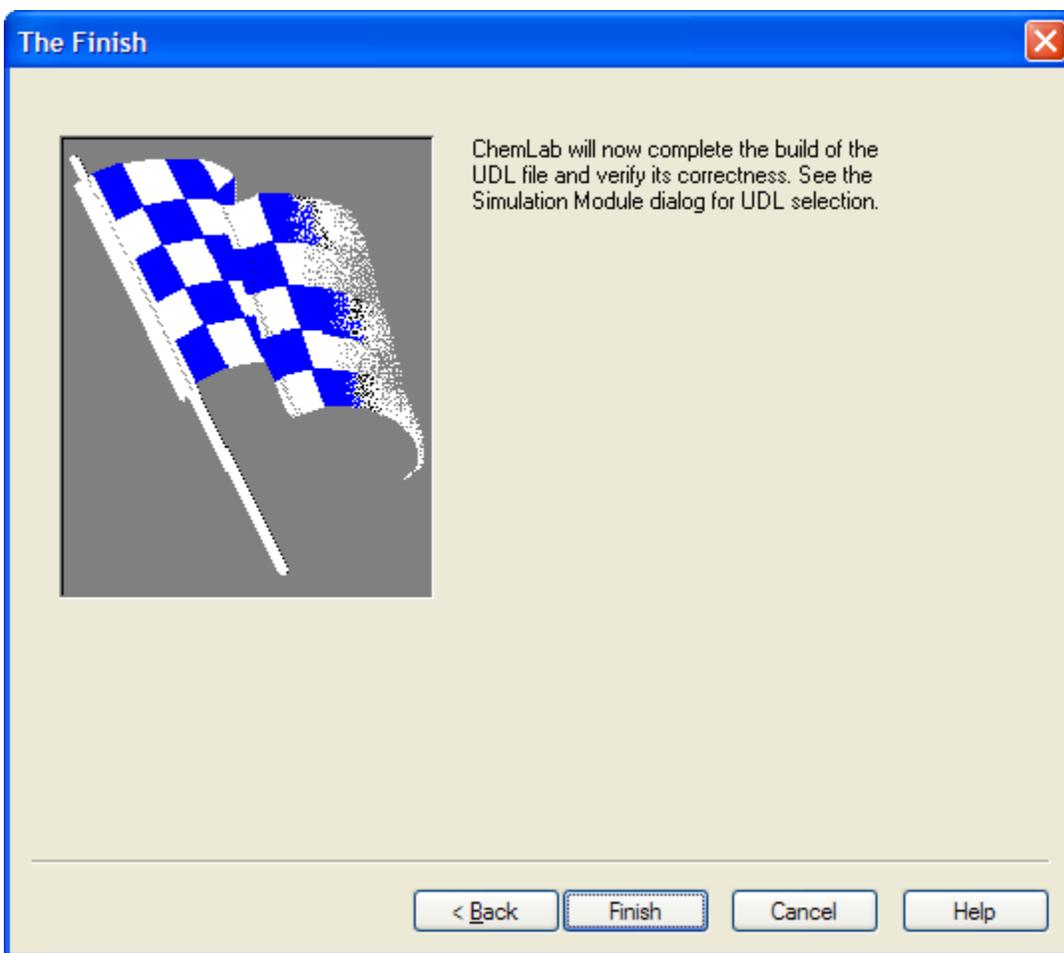


1. Attached PDB Files for Molecular Viewer: List all the chemicals in a lab simulation and any associated PDB files.

2. Select PDB File...: When a chemical is highlighted the “Select PDB File...” button will become enabled. Pressing the button will open a file dialog. The user then uses the file dialog to attach a PDB file to the highlighted chemical.
3. Clear PDB File: Allows the user to remove a PDB file associated with the highlighted chemical.

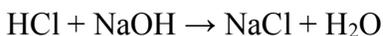
Finish Screen

This is the final screen, pressing finish will create the UDL file and load it into ChemLab. The UDL file will be added to the working directory of ChemLab and will now appear in the Lab Simulation Modules dialog box.



Strong Acid and Base Lab Example

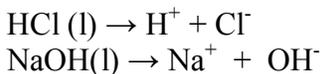
When an acid and a base react, the net result is the production of a salt and water. In this experiment, NaOH will neutralize the HCl in a reaction that produces sodium chloride (salt) and water:



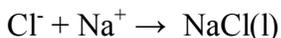
If we only enter this neutralization reaction into the Lab Wizard, we would not obtain the expected result, that is, a slowly rising pH with a sharp rise in pH near the end point when NaOH neutralizes the HCl. This is because this formula does not take into account the equilibrium reaction that occurs when water dissociates into H^+ (hydrogen ion) and OH^- (hydroxide ion).

The dissociation of water reaction can be expressed as:
 $\text{H}_2\text{O} \leftrightarrow \text{H}^+ + \text{OH}^-$ with an equilibrium constant $k = 1 \times 10^{-14}$

Since the acid and base are both strong, we can assume they dissociate completely when mixed with water:



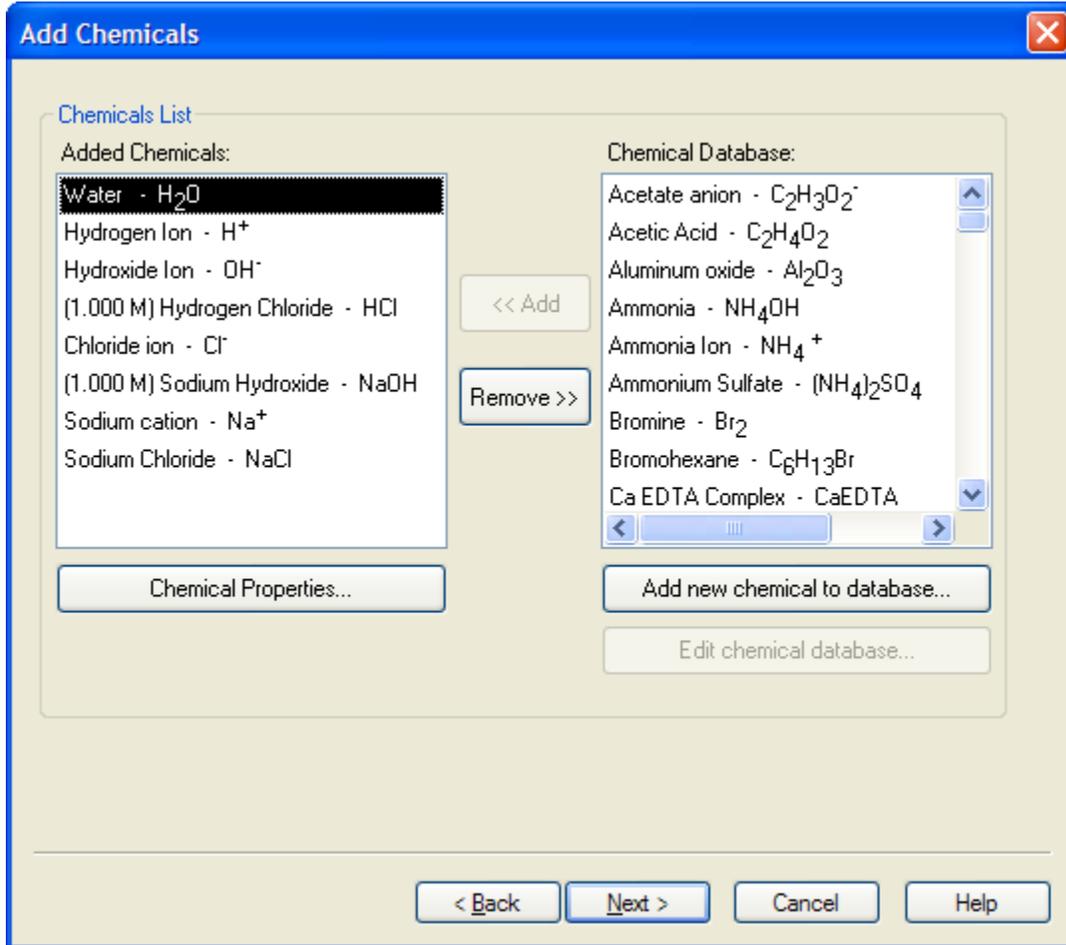
Finally, the reaction of chlorine and sodium ions to produce a salt can be expressed as:



Hence, for this lab we will need the following chemicals:

- Water (H_2O): a stock chemical
- Hydrogen Ion (H^+): reaction product
- Hydroxide Ion (OH^-): reaction product
- 1.0 M HCL: stock chemical in 1M solution
- Chloride ion (Cl^-): reaction product
- 1.0 M NaOH: stock chemical in 1 M solution
- Sodium cation (Na^+): reaction product
- Sodium Chloride (NaCl): reaction product

Add Chemicals screen with chemicals for neutralization of HCl with NaOH:



Add Reactions dialog with reactions added for dissociation of Water, HCl and NaOH and reaction of Na⁺ and Cl⁻.

Add Reactions

Reaction Tree:

- Reactions
 - Dissociation of Water
 - Reactants
 - Water
 - Products
 - Hydrogen Ion
 - Hydroxide Ion
 - HCl dissociation
 - Reactants
 - Hydrogen Chloride
 - Products
 - Hydrogen Ion
 - Chloride ion
 - NaOH dissociation

Available Chemicals:

| Available Chemicals | Type |
|---------------------|---------|
| Water | Stock |
| Hydrogen Ion | Product |
| Hydroxide Ion | Product |
| Hydrogen Chloride | Stock |
| Chloride ion | Product |
| Sodium Hydroxide | Stock |
| Sodium cation | Product |
| Sodium Chloride | Product |

1.000 (H₂O) -> 1.000 (H⁺) + 1.000 (OH⁻)
(LHS = 18.015, RHS = 18.015)

Add Reaction... Edit Reaction... Delete Reaction Edit Chemical...

< Back Next > Cancel Help

Reaction Details for the dissociation of water. Note that the chemical equilibrium setting is used and that the reaction is instantaneous.

Reaction Details ✖

Reaction Name:

Requires Heating Minimum Temperature: °C
 Requires Stirring Maximum Temperature: °C
 Requires Light

Use Heat of Reactions: KJ
 Use chemical equilibrium:

Reaction Rates

Instantaneous
 Fixed Rate, zero order in [A] & [B], $d[A]/dT$: Rate varies with concentration: k: m:

Where: $A+B \rightarrow C$, represents the reaction

Lab Options screen, where the “Include pH meter” option must be set in order that pH values can be displayed and a titration curve plotted.

Lab Options

Acid Base Lab

Include pH meter

Solubility

UDL Simulation handles all solubility reactions (ignore chemical database solubility values)

Spectrophotometer

Include Spectrophotometer Add/Edit Spectrophotometer Data...

Thermodynamics

Include Calorimeter Include Temperature in Titration Plot

< Back Next > Cancel Help