General Instructions for Running the Virtual ChemLab Program

Entering the program: First, log onto the network using your student ID and password. Virtual Chemlab is listed under "All Programs." Enter the program by then clicking on the "Organic Chemistry Laboratory" door. The password is "chemlab" (and for some reason it must be typed slowly).

Choosing a reaction: Go to the stockroom. Click on the keyboard, then choose the appropriate reaction. This fills the bottles on the stockroom shelf with starting materials for that reaction. You don't have to repeat this step if you are running the same reaction again.

Setting up a reaction: In the stockroom, drag a round bottom flask over to the cork ring. Then double click on the reagent(s) and solvent that you want to add. They are automatically added in appropriate amounts. (Note – if you can't drag a flask over, it is probably because you already have a reaction going. In order to start over, you must double click on the red waste container in the lab).

Adding reagents: Go back to the laboratory. The flask with your reagents is now sitting on the stir plate. You can now add any of the reagents from the bottles on the lab bench by double clicking. Choose the one that is appropriate for the reaction you are performing.

Running the reaction at room temperature: If you want to run the reaction at room temperature, simply double click on the N_2 tube (all reactions in this simulation are run under nitrogen to prevent contamination by water or oxygen).

Running the reaction at reflux: If you want to heat the reaction, click on the drawer labeled "heater," then double click on the heating mantle (this is an old-fashioned way to heat a reaction before spark-free stir-hot plates were available). Then click on the drawer labeled "condenser" and double click on the reflux condenser to hook it up. Close the drawers again by clicking on them. Then double click on the N_2 tube.

Running the reaction in an ice bath: If you want to cool the reaction, double click on the ice bucket, then double click on the N_2 tube.

Starting a reaction: To start the reaction, click on the stirrer/hot plate.

Help screen: To see what is in the reaction mixture, click on the handle in the upper right hand corner. A screen will come down showing a list of all chemicals present in the reaction, including products if any form. Starting materials will disappear when they are used up. The structure for each chemical will appear on the chalkboard if you put the cursor over the name on the help screen.

Clock: To advance the time, click on the part of the clock that you want to advance (hour, 10 minutes, or 1 minute). The clock will also advance automatically every time you perform an operation like TLC or IR.

TLC: To take a TLC of the reaction as it runs, drag a TLC from the jar to the reaction. The first column is always the starting material, the second is the reaction. 20% ethyl acetate in hexanes is used as the eluting solvent. If the starting material or products do not appear, it may be because they are not UV active, or they are so volatile that they evaporate off of the plate while it is running.

Stopping the reaction: When you want to stop the reaction, open the drawer labeled "separatory funnel" and double click on the funnel. This puts the funnel on the ring stand and transfers your reaction to it.

Extraction: Before doing any further characterization, you must add one of the water solutions at the right hand side of the bench (H_2O, 0.1M NaOH, or 0.1 M HCl). Clicking on one of the bottles adds the solution plus a layer of ether to your reaction mixture and shakes it up (not shown). By putting the

cursor over either solution, the help screen will tell you what it contains. Any compounds that are highly volatile will evaporate during the extraction.

Drying and rotovapping: To dry and rotovap the organic layer, or rotovap the water layer, simply click and drag either one to the bench.

Taking an IR: You can now take an IR by dragging a salt plate from the IR machine (back left corner of the lab). An IR spectrum will appear on the screen.

Taking an NMR: You can take an NMR by dragging an NMR tube from the NMR machine (back right corner of the lab). An NMR spectrum will now appear on the screen. You can expand any portion of the spectrum by clicking and dragging over the peaks of interest. Go back by clicking on "zoom out." The peaks are numbered from left to right, and the integration is given under the title of "height" (meaning height of the integration line) in the table below the spectrum.

Distillation and boiling points: To purify a liquid or separate two liquid compounds you can use a distillation. First place the flask on the stir plate. Then click on the drawer labeled "distillation" and drag the distillation apparatus to the flask. Make sure to double click on the N_2 tube so that the apparatus isn't heated under pressure. It takes 10 minutes to heat the liquid to boiling. If you place the cursor over the thermometer at the top of the apparatus, you can see the boiling point of the liquid being distilled. You can take IR's, NMR's, or TLC's while the distillation is occurring.

Recrystallization and melting points: In order to measure a melting point, a solid must first be purified by recrystallization. First, click on the drawer marked "crystallization" and double clicking on the dish to place it on the stir plate. Next, drag the flask containing the solid to be crystallized to the dish. The compound is now pure enough to take a melting point by dragging a melting point tube to the dish. Placing the cursor over the apparatus will bring up the display. If it reads "*.*" then the mp is below 25^{o} C. If you take a melting point of a mixture of solids, it will average them.

Cleaning up a reaction: When you have finished with a reaction, double click on the red waste disposal bucket (under the stockroom window), and presto, everything is cleaned up for you. You can now go to the stockroom to start a new reaction or exit the program.

Exiting the program: To exit the program, click on the "exit' sign above the door.