Step-by-Step

Creating and Running a Simulation in ActivChemistry

Using ActivChemistry, you can create simulations that represent real-life scenarios in chemistry. This Step-by-Step Card introduces you to the elements of ActivChemistry, identifying the most important tools for creating chemistry simulations.

Creating a new simulation

1. Open the ActivChemistry application.
2. Choose New Simulation from the File menu.

Creating and placing objects

1. Open the Components menu to view the following submenus, which incorporate a wide variety of simulation elements:
   - **Atomic –** Parts of an atom
   - **Calculators –** Mathematical functions to help you evaluate results
   - **Electricity –** Electrical components such as batteries and light bulbs, as well as electric meters
   - **Equipment –** A wide variety of containers and heating elements
   - **Logic Components –** Timers and tools to manipulate values
   - **Measuring Devices –** Devices to measure any part of your simulation, with the exception of electrical values which are available in Electricity
   - **Recorders –** Tools to graph or save results
   - **Resources –** Labels and reference materials you can place in your simulation

   You can select any of these submenus to see a list of objects. For example, if you choose Equipment, one of your choices is a Big Bottle.
2. To place an object inside your simulation, choose it by selecting one of the objects from a submenu. Then move the pointer inside the window titled Workbench. The pointer looks like a stamp ().

3 Click where you want to place the object.

Creating atoms

Normally, creating and placing an atom places a randomly-selected atom each time you click the Workbench. However, you will probably want to place an atom that you choose. To place a specific atom, follow these steps:

1 Open the periodic table. Choose either Large Periodic Table or Tiny Periodic Table from the Windows menu.

2 Select the atom of your choice by clicking it.

3 To use a randomly selected atom, click the upper-middle portion of the periodic table, which is either blank or shows information about the selected molecule.

4 To place your atom, click the desired place in your Workbench.

5 To close the periodic table, click the periodic table window close box. Your currently selected atom stays selected.

Moving objects

You can move objects around the Workbench, and you can also place objects onto a shelf to get them out of the way or to save them for later use.

1 To move an object, select the hand tool  from the toolbar at the top of the screen.

2 Position the pointer on the object you want to move.

3 Drag the object to the new location inside the Workbench, and release the mouse button.

Using objects

Some objects have special features. Select the hand tool  to utilize these features. There are three uses for the hand tool in addition to moving objects.

- **Activating objects –** Clicking the neck of a bottom puts a stopper in it or takes it out.
- **Using buttons –** Several objects contain buttons, such as up and down arrows or units. Click these buttons to modify settings.
- **Other settings –** Double-clicking changes settings on selected objects. For example, you can change the value of a constant or the message on a label.

Removing and emptying objects

1 To remove or empty an object, select the sponge tool  from the toolbar.

2 Click the object you want to remove or empty. If the object is already empty or does not contain anything, it is removed.

3 If you want to only partially empty an object, hold down the Option key on your keyboard while clicking the object. You are asked to enter an amount.

Using shelves

You can use shelves to store objects. Any kind of object, with the exception of atoms and molecules, can be placed on a shelf.

1 To create a new shelf, choose New Shelf from the File menu.

2 To place a copy of an object in your Workbench onto a shelf, select the hand tool  ; then drag the object from the Workbench onto the shelf.

3 To place a copy of an object from a shelf into your Workbench, select the hand tool  ; then drag the object from the shelf onto the Workbench.

4 To remove an object from a shelf, select the sponge tool  ; then click the object on the shelf.

Linking objects

There are a variety of objects that can be linked together. For example:

- **Atoms –** Atoms link together to form molecules. Link an oxygen molecule to two separate hydrogen molecules to form water.
- **Equipment –** Heaters and other tools can be linked to containers or test tubes.
- **Measuring devices –** You can link a piece of equipment or an electrical tool to a measuring device.
- **Logic components and records –** These devices link to measuring devices or additional logic components.

Make sure you link objects in the correct direction. Linking objects in the wrong direction or linking incompatible objects together will result in an error message describing why the link was unsuccessful.

1 To link two objects together, select the link tool  from the toolbar.

2 Position the pointer on the object you want to link to another object; then drag over the object you want to link this object to, and release the mouse button.

Using the eyedropper

The eyedropper can pick up stray atoms and molecules, or those residing in a container. It can then place copies of them on the Workbench or add them to a container.

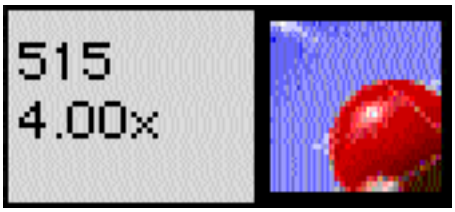
1. To pick up atoms or molecules, select the eyedropper tool  from the toolbar.
2. Click the atom or molecule you want to pick up, or click the container they reside in.
3. Click the place on the Workbench or the container in which you want to place the atom or molecule. If you place it in a container, it will place a large quantity of that particular atom or molecule.
4. To add a specific mass of atoms or molecules to a container, hold down the Option key while clicking the container. You are asked to enter an amount.

Ionizing atoms

1. To ionize an atom, select the ionize tool  from the toolbar.
2. To add an electron to an atom, click the atom.
3. To remove an electron from an atom, hold down the Option key while clicking it.

Changing the zoom factor

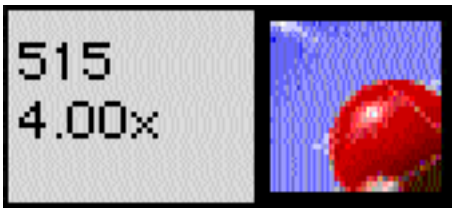
You can zoom in and out in the Workbench. This does not change the size of objects shown. Instead, it changes how far apart they are. The current zoom factor is shown on the right side of the toolbar at the top of your screen. It is the number shown on the bottom (4.00x in this example):



1. To zoom in, choose Zoom In from the Options menu. You are limited to a maximum zoom factor of 4.
2. To zoom out, choose Zoom Out from the Options menu. You are limited to a minimum zoom factor of 1/4.

Running a simulation

When you have finished setting up all of the elements of your simulation, you will want to run it. The duration of simulation is measured in clock ticks. The current clock tick is shown on the right side of the toolbar at the top of your screen. It is the number shown on the top (515 in this example):



- To run a simulation, click the run/stop button on the toolbar.
- To stop a running simulation, click the run/stop button again.
- To run a simulation for a single clock tick, click the single step button.
- To revert the simulation to its state at the last checkpoint, click the rewind button. The default checkpoint is every 50 clock ticks. You may not rewind beyond the last checkpoint.
- To change the default checkpoint, choose Preferences from the Options menu. Click the box on the left titled "General." Enter a new checkpoint value in the Workbench portion of the window next to "Checkpoint every."
- To revert the simulation to its state before the last run, choose Undo from the Edit menu. You may only undo the very last run.

Saving simulations and shelves

You may want to save a simulation for later use, or save single objects from your experiment.

- To save the current simulation, choose Save Simulation from the File menu. Type a name and select a location where you want to save the file.
- To save the currently open shelf, choose Save Shelf from the File menu. Type a name and select a location where you want to save the file.

Opening saved simulations and shelves

- To open a saved simulation, choose Open from the File menu. In the lower portion of the window, click the button next to Simulation. Locate the folder in which you saved your simulation, select it, and click Open.
- To open a saved shelf, choose Open from the File menu. In the lower portion of the window, click the button next to Shelf. Locate the folder in which you saved your shelf, select the shelf, and click Open.