# Chem 260 Laboratory 2

This lab provides experience with 3-dimensional plots in Excel. Although it is cumbersome to set up 3-D plots in Excel, and the plotting routines are not very sophisticated, it does allow you to view a surface from any angle or perspective. We will explore the nature of a potential energy surface in a future lab. For now, however, you will practice with simpler, more familiar functions – the wavefunctions for a particle in a 2-D box. Symmetry is an important aspect of this lab.

The second part of the lab uses HyperChem to look at various aspects of molecular and orbital symmetry.

**Warning**:
Save your work frequently, or suffer the consequences when your workstation crashes! When you need to copy a plot to your Word document, use Edit/Paste Special and paste as a picture (or enhanced metafile). If you paste a large 3-D plot as an Excel object you are asking for trouble.

## WAVEFUNCTIONS FOR A PARTICLE IN A 2-D BOX

1. Copy the file 260lab2.xls from the network drive to your local hard drive. Open it in Excel. Beware! This is a large file and it is easy to overload your computer resources if you have other programs running at the same time.
2. Look at the different pages: Data, 3-D Plot, and Contours. Notice the relationship between the 3-D plot and the Contour plot. The colour coding for the *z*-axis ranges is given in the legend on the Contour page.
3. Try changing the quantum number n from 1 to 2. Observe the shape of the wavefunction.
4. You can rotate or tip the 3-D plot by selecting one of the corners of the box and dragging it with the left mouse button.
5. Another way to change the 3-D view is with Chart/3-D View. If you use this with the Contour plot you can see that this is really just a 3-D plot viewed from a particular perspective.
6. Try a few other combinations of the quantum numbers n and m. Paste the 3-D plot and Contour plots for the state n = 2, m = 3 in your report.
7. Now alter the spreadsheet so that you plot the *square* of the wavefunction. Change the z-axis so that it has a lower limit of 0 and has 10 major divisions. Don't forget to change the axis title!
8. Plot $(\psi/N)^2$ for the state n = 2, m = 3 and paste into your report.
9. By inspection of your plot(s), calculate the probability that the particle is in the region $0.250 \le (x/a) \le 0.750$ and $0.167 \le (y/b) \le 0.500$. Report your answer in your lab report.
10. Close Excel before you start the next part of the lab, or your computer might run out of memory.

A SQUARE MOLECULE

1. Start HyperChem Lite. Construct the cyclobutadiene molecule. Start with the draw tool (top left icon). Click and drag. You probably get $H_2$. Click on one H and drag, let go, click and drag until you have drawn a square. The H's should now be C's, since carbon is the default element. If necessary, change the default with Build/Default Element. Click on one C-C length to make it a double bond. Make the opposite C-C bond double. Build/Add Hydrogens and Build/Model Build.
2. Optimize the structure using Molecular Mechanics. Use the various rotation tools to inspect the molecular shape. Try different rendering (Display/Rendering). In particular, try shaded spheres. Notice the planar shape of the molecule.
3. Return to the stick display and orient the molecule so that it looks like the original square.
4. Perform a single point EHT calculation and Compute Orbitals. Note that there are two degenerate levels at the HOMO level. (HyperChem's Labels command puts two electrons in one orbital and none in the other, but we know better – there ought to be one electron in each degenerate orbital.)
5. Plot the HOMO. Cut and paste it to your lab report.
6. Select the degenerate level, plot its orbital. Cut and paste to your report. Compare with the degenerate orbital.
7. Repeat for the LUMO. Notice the orbital nodes. How many are there?
8. Are you sure? Rotate the molecule out of plane so that you see the 3-D representation of the orbital. See the extra nodal plane through the nuclei. Orbitals with such a plane are $\pi$ orbitals.
9. For examples of orbitals of $\sigma$ symmetry inspect the degenerate pair of levels immediately below the HOMO level. Notice again the relationship between symmetry and degeneracy.
10. For another pretty $\sigma$ orbital look at the level (HyperChem Number 13) just above the LUMO.