

Plotting Radial Wavefunctions

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Learning Objectives:

1. Learn how to extract data from all electron plots.
2. Use Xmgrace to plot radial wavefunctions for s , p and d orbitals.
3. Learn how to extract the probability density plot through manipulation of Xmgrace.

You should have completed the first two OPIUM tutorials before getting started. Any other assigned elements should have at least the all-electron (AE) calculations complete and the wavefunctions plotted. If you haven't done that, go back and do that now. You may need to create files for additional elements so you can plot the radial wavefunctions for the 1-6 s orbitals, the 2-6 p orbitals and the 3-5 d orbitals. We will *NOT* be plotting the f orbitals, but you're more than welcome to try that on your own time.

Extracting Data From Xmgrace Plots

First, if the plot you want to extract data from isn't open, you can open it from the command line. For example, if we want to open the AE wavefunction plot of Hydrogen, we would type: **xmgrace H.ae.gr**

A new window should pop up on the screen showing the plot. To extract the data, you want to click on the "Data" option along the top of the xmgrace window. Then click on "Export" and then on "ASCII". The first data set will be s dataset (Hydrogen only has one), and in the selection box, type: **1s.dat** Once done with your plot, exit out, and check to make sure you correctly extracted the data. Typing the command **ls** will give you all the files in the directory. If you correctly copied the data over, you should see a file called 1s.dat listed.

In files containing multiple valence orbitals, the first dataset should be the s data, the second dataset, the p , and the third dataset, the d . For example, in Carbon, the first data set is the $2s$ and the second dataset is the $2p$.

Repeat these steps for to obtain data files for the $2s$, $3s$, $4s$, $5s$ and $6s$ AE wavefunctions and also for the requested p and d wavefunctions of various elements before moving on to the next step.

Plotting Radial Wavefunctions

We're going to make a total of four plots now. The first plot we're going to make is going to include all of our s radial wavefunctions. We can do this by typing the following in the command line: **xmgrace 1s.dat 2s.dat 3s.dat 4s.dat 5s.dat 6s.dat**

To adjust the axes, and to label the axes and the graph, we want to click on the "Plot" option at the top of the window. If one clicks on "Axis properties", one can change the axis range, label the axis, change the spacing between tick marks, etc. If you switch it from "X axis" to "Y axis" you can also adjust the other axis. Exit out when finished.

To change the colors or thickness of the lines in the plot, you'll go back to "Plot" at the top of the window and then click on "Set appearance". Select the data set you want to change (and this is why you want to string them in order), label it, and increase the line thickness as desired. Color of each set can also be changed if desired—make sure each set is a different color! Once this is completed, exit out of the sub-window.

Next, go back to "Plot" and click on "Graph appearance". This is where you will title your graph and move the legend around. Again, when finished, exit out of the sub-window. Once you're happy with how your graph looks, save it. To do this, click on "File", then on "Save as". Don't click on save, as this will rewrite one of your data files! In the selection window, type a name for your plot in, for example **AE_s.agr**. Once done, click OK, then go back to "File" and click on "Print setup". Change your device from the default of "Postscript" to "JPEG". Enter a name for your file, and increase the resolution if desired. Once this has been completed, copy to the your local desktop.

Make plots for the p radial wavefunctions, the d radial wavefunctions, and then all of the radial wavefunctions. Once all of them are completed, email them to yourself or your lab partners so they can be included in your lab report, and answer the following questions (answers should be in both your lab notebook and the report).

1. What is the relationship between the principle quantum number and the number of nodes

in the radial wavefunction?

2. How do the s , p and d radial wavefunctions differ?
3. What is the relationship between atomic radius and principle quantum number?

Obtaining Probability Density Plots

To plot the Probability Density, we need to have the the absolute value of the radial wavefunction squared, $|\Psi(\hat{r})|^2$. Open up your AE.s.agr file by typing the following in the command line:
xmgrace AE.s.agr

Once the window containing the plot pops up, click on "Data", then on "Transformations", and then on "Evaluate expression". Select the set or sets you want to perform the transformation on. To calculate $|\Psi(\hat{r})|^2$, type **y=sqr(y)** in the formula box. Click "Apply". This should be done for all sets, but do not apply multiple times, as this will keep repeating the formula! **How do these results relate to the Pauli Exclusion Principle?**

Having constructed our OPIUM files and our plots, we should now be able to do a comparison of the orbital energies. We should now be able to interpret the trend that we know of as the Aufbau Principle. This trend arises from the planar nodes in the orbitals, and forces the electrons in higher n states to spend an increasing amount of time further from the nucleus. **How do you think this affects the attractive electrostatic field? It may help to recall Slater's Rules**

Answer the following questions using the class data and put them in your lab report.

1. **Use the eigenvalues (energies) of the valence s , p and d states of at least six elements going across a period of your choice in the periodic table.**
2. **How to E_s and E_p trend across a given period and why?**
3. **How does the $E_s - E_p$ trend from right to left across the periodic table? What do you think this means in terms of an atom's ability to hybridize s and p electrons?**