

Investigating Atoms and Ions with Computers:

The Aufbau Principle and Periodic Trends

Overview

Every student who has ever taken a chemistry course is familiar with the periodic table and has learned how to read it. Elements are organized by increasing atomic number, and each group contains elements possessing similar chemical behavior. Various trends are also associated with the periodic table, and many of these trends, are often memorized rather than understood. This series of activity seeks to introduce computational chemistry by utilizing it to increase comprehension of electron configurations, the Aufbau principle and periodicity for first-year students. This exercise will utilize the Open-Source Pseudopotential Interface/Unification Module (OPIUM) and Xmgrace to determine correct electron configurations, examine the relationships between quantum numbers and radial nodes, to question the Aufbau Principle and to inspect trends in periodicity.

Pre-laboratory Questions

Must be written in your lab notebook and turned in prior to the start of class.

1. What are the electron configurations for your assigned elements? How many total orbitals are in each configuration for each element?
2. For one of your assigned elements with quantum number $n=3$, what other electron configurations are you planning on testing? Write the configurations for each of them. Why do you want to test these configurations?
3. For one of your transition metals, write the electron configurations for the neutral atom, the +1 cation, and the +2 cation. How many total electrons do each of these have?
4. Find the literature values for the first and second ionization energies for the element you chose in number 3. Record these and your source.
5. Determine the conversion factors to convert Ry/atom to kJ/mol.
6. What is the formula for determining percent error?

Objectives

In this experiment, you will

- Gain experience with open-source computational chemistry software.
- Identify relationships between quantum numbers, atomic orbital energies, and wavefunctions.
- Learn how quantitatively identify incorrect electron configurations.
- Determine if and where exceptions to the Aufbau Principle occur.
- Calculate ionization energies and compare with literature.
- Extract and plot trends from quantitative data.

As this activity will require 2 laboratory periods, it is broken into two parts: Investigating the Aufbau Principle and Periodic Trends

Materials

Lab computers with OPIUM and Xmgrace installed either in Linux or on a Virtual Machine

Periodic Table

Directions on how to use OPIUM and Xmgrace

Methods

Investigating the Aufbau Principle

1. Log in to the computer, then log in to the server or access the virtual machine as directed by the instructor.
2. Follow along with the instructor to work through the Hydrogen and Carbon lessons. Record data as directed.
3. From the plots created, copy the required data to a .dat file or Excel. Directions on how to do this are provided on Canvas.
4. Complete all-electron calculations for all assigned elements and record your data.
5. To run different configurations of an element or ion, there are two approaches. If you want to change the entire configuration, create a new input file.
6. To change only the valence electrons, add a fourth keyblock to your input file. This keyblock is called [Configs]. Using this allows one to run calculations for different configurations or ions in one file. For example, to do so for carbon, add the following at the end of the input file:

[Configs]

```
2          ---how many test configurations are being examined
#          ---separates the different configurations
200 2.00 -  ---first valence orbital in the test configuration, it's filling, & energy guess
210 2.00 -  ---second valence orbital in test configuration, filling, & energy guess
#
200 1.00 -
210 3.00 -
```

In this case, one would be examining how changing the electron configuration affects the valence orbital and total energies. One can test as many test configurations as one desires.

7. Run a variety of different configurations for one of your assigned elements in period 3. For the configurations you tested, **how can the correct electron configuration be identified?** (Data Analysis Question 1) Explain your reasoning. (Because the book says a particular configuration is correct is not a valid answer.)
8. Create a graph for one of your non-transition metal elements showing the orbitals filling in increasing energy. The x-axis should be your orbitals in nlm notation, and your y-axis should be the energy of the orbitals in Ry. Label your graph.
9. Create a graph for one of your assigned transition metals. The graph should have the same axes used in 8.

At this point, you should be wrapping up week 1 of the lab. Next week will wrap up Part I by examining the relationship between quantum numbers and radial nodes, and will then continue on with Part II. Turn all data from Week 1 into the instructor so the class database can be completed and uploaded to Canvas.

10. Compare your graphs from 8 and 9. And, using the class data, create a plot of $4s$ and $3d$ orbital energies for the 3d transition metals. Label your graph. What happens as one moves from left to right across the period? Do all of these follow the diagram in the text?
Is the Aufbau Principle obeyed in all circumstances? (Question 2)
11. Plot a graph plotting the radial wavefunctions for the $1s$, $2s$, $3s$ and $4s$ orbitals. (Use the directions for plotting in Xmgrace/Excel found on Canvas) **How are quantum numbers and radial nodes related?** (Question 3)
12. Plot the radial wavefunctions for the $3s$, $3p$, and $3d$ orbitals. **Within a particular quantum number, what is the relationship between radial nodes and type of orbital?** (Question 4)

Periodic Trends

13. To calculate the first ionization energies, run all-electron calculations for the neutral atom and for the +1 cation for one of your assigned metal atoms. Record the total energy for each.
14. Take the difference between the total energy of the +1 cation and the neutral atom. As all of the energies provided by the software are in Ry/atom (electron), unit conversions will be necessary to convert to the SI units students are familiar with. **How is ionization energy related to energy?** (Question 5)
15. Calculate your percent error. Literature values can be obtained from the textbook or from the NIST Chemistry Webbook.
16. To calculate the second ionization energy, run the all-electron calculation for the +2 cation. Take the difference between the +2 cation and the +1 cation's total energies. Convert to SI units. Calculate the percent error.
17. Make a table of containing the valence orbitals and their energies for the representative elements. **Can atomic orbital energy provide insight on electron affinity?** (Question 6)
18. Examine the class data, **does the data explain why elements seek noble gas configuration?** (Question 7)
19. All tables and graphs must be in your typed, electronically submitted lab report.

Data Analysis Questions

Investigating the Aufbau Principle:

1. How can the correct electron configuration be identified?
2. Is the Aufbau Principle obeyed in all circumstances?
3. How are quantum numbers and radial nodes related?
4. Within a particular quantum number, what is the relationship between radial nodes and type of orbital?

Periodic Trends:

5. How is ionization energy related to energy?
6. Can atomic orbital energy provide insight on electron affinity?
7. Does the data explain why elements seek noble gas configuration?

Error Analysis

Discuss the percent error found from your ionization energies. What do these values tell you about the methods used by the software?

Conclusion

How has your understanding of electron configurations changed after doing this lab? Were you able to meet all of the objectives? Are there any parts of the exercise you would like to spend more time on or that are still unclear?