Preliminary Activity for Investigating Atoms and Ions with Computers! Part II: Periodic Trends

The primary objective is to learn how to calculate ionization energies and to extract periodic trends through tabulating and plotting data. This activity is designed to build off of the previous activity, Investigating the Aufbau Principle. You and your classmates will continue to build a class database, and will examine how the total energies of atoms and cations can be used to calculate ionization energy. Please refer back to the materials utilized in the Preliminary Activity during week one to refresh on software operations and the use of the [Configs] keyblock.

To calculate ionization energies, one would take the difference between 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. Literature values can be obtained from the textbook or from the NIST Chemistry Webbook.

Questions

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

Note:

The plan you submit for obtaining ionization energies must include the electron configurations for both the neutral atoms and cations you plan on testing for your selected assigned elements. Include the commands needed for the software and unit conversions required to convert Ry/atom to kJ/mol. Also explain how data will be organized.