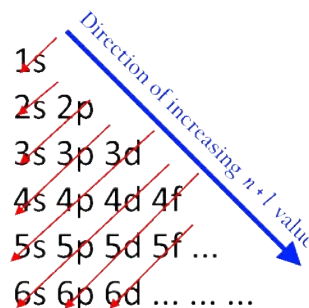


1 Aufbau principle

Quantum numbers are a handy way to account for the electrons that fill up atomic shells, but they can be tricky to keep track of. Instead, we often utilize shorthand to label the quantum numbers:



The Aufbau principle is a trick to keep track of the order each subshell is filled in:

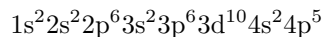


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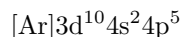
The superscript after each subshell indicates the number of electrons in the subshell: each should be full except for the outermost shell, which is filled based on the number of valence electrons.

Example: Write down both the full electronic configuration and the noble gas notation of Br.

Br has 35 valence electrons, so we can fill up all the way to Argon. The full configuration, which mostly follows Aufbau, is



Note here that the $3d^{10}$ and $4s^2$ occur in an unexpected order: there are some exceptions to the Aufbau principle. We don't expect you to memorize these exceptions for 3.091, but know that they are noted in the periodic table! The noble gas configuration just shows the electrons beyond the last full shell:

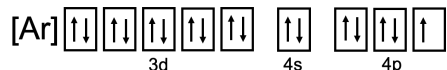


2 Electron filling and box notation

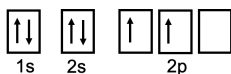
We can note the configuration and orientation of the electrons visually using box notation. It's usually easiest to use the Aufbau principle (or the periodic table!) to write down the electronic configuration and then translate it to box notation. It's important to recall *Hund's rule*: every orbital in a subshell must be singly occupied before any orbital is doubly occupied.

Example: Draw the electronic configuration of Br and C in box notation.

We wrote the noble gas configuration above, so we can just give the box notation of the valence electrons here:



For carbon, the electronic configuration is $1s^2 2s^2 2p^2$. In box notation, we fill up the 1s and 2s states, and populate the 2p according to Hund's rule:



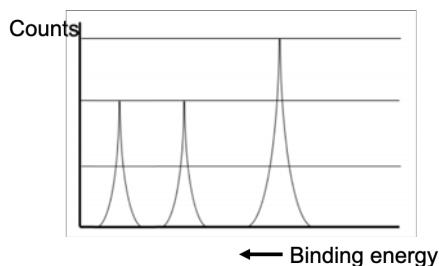
3 Photoelectron spectroscopy (PES)

Photoelectron spectroscopy (PES) is an experimental method used to determine electronic structure. First, a sample is bombarded with high energy photons to ionize the atoms. Then, the kinetic energy of the electrons that are emitted is measured. The binding energy can be determined using

$$E_{\text{binding}} = h\nu - KE_{e^-}$$

By plotting the relative counts of electrons emitted with various binding energies, the elemental composition of a sample can be determined using PES!

Example: Determine which element corresponds to the following PES spectrum:



On this plot, the binding energy increases to the *left*. The electrons closer to the nucleus should have the highest binding energy, so the left-most peak must correspond to the 1s electrons. The relative height of the peak corresponds to the relative frequency at which the electrons are emitted: since there are two 1s electrons, the height of the left-most peak must correspond to two electrons. The middle peak must correspond to two 2s electrons. Then, since the right-most peak is 1.5 times taller, it must represent 3 electrons in the 2p subshell. The electronic configuration for the element in this PES diagram must be $1s^2 2s^2 2p^3$, which corresponds to nitrogen.

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