MSE 110 Project

Program 1: This program, which was took its base from the phase diagram program that was already written provides phase diagram data for tungsten oxides, of which there are several. I made this program because we have element tungsten in our lab, and it is a good habit to do PXRD (or pseudo-PXRD in the case of foils or rods) to make sure that your starting material is the "pure" elemental material. If it is not, particularly in the case of metal oxides in foils or rods, there will often be a build up of oxides on a surface layer that can be removed by mechanical weathering (sanding, filing, cutting). After this is done, it is always a good idea to check and see if the surface shows a good XRD pattern for a bulk material (we would check against ICDD patterns), but it is also good to know what the stable forms of the oxide are so that you can check both for tungsten (your desired material) as well as WO_2 and WO_3. Therefore, the program draws from the Materials Database for the phase diagram data, and then provides the XRD patterns for the most stable materials (which are W, WO_2, and WO_3). This script could easily be re-written for any element and its oxides, making it quick to allow for a check on the quality of the material before handing it over to a user. It could also be changed to allow for checks on things like metal hydrides if a user was looking for say, an elemental lanthanide; several of these elements are known to act as hydrogen sponges and so have to be heated in an inert environment to quite high temperatures to vaporize the hydrogen which is often located interstitially throughout the lanthanide lattice.

Program 2: This program displays the neutron scattering cross sections (total and absorption) for the rare earth elements, which are of particular interest for metal hydrides and battery materials among other things. We are constantly wondering about the scattering cross sections of various elements in order to try and figure out illumination times in the beam, and so I figured this would be a handy script to have to visually depict the scattering and absorption cross sections. Knowing absorption cross section is also quite important to try and understand how activated a sample is—an element that absorbs neutrons will come out quite "hot" and thus the sample will need to sit for a long to de-activate before we can take it off of the sample stick. This program draws from another database which has a GitHub repository that I cloned to be able to interact with it. It has a kind of complicated system for calling, and it took a lot of trial and error, reading the "Read the Docs" page, and help from Gemini (Google's AI) in order to figure out how to call the appropriate attributes to get the scattering cross sections I wanted.