Chem-6111 Homework 1

Data Analysis and Acquisition, CU Boulder, Fall 2012

Due before class on 6 Sept. 2012 by submission to the d2l dropbox

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NOTES

1. You must report the results (text and/or graphs) of your work in a Notebook in the experiment. This is the work I will grade. I will not search for additional graphs in your experiment.
2. You should keep the waves for each question in their own DataFolder (this will make it easier for me to look at your work).
3. Please follow the programming style conventions (on the course website). You will receive points for following these guidelines. These are especially for your benefit – they help make your code clearer and easier to understand after you come back to it after a while. Remember, "write code for the reader!"

Question 1: Speed Distribution of Gas Molecules

Write a function to calculate the Maxwell-Boltzmann distribution of speeds given the mass of the moving object, the maximum speed for consideration, and the temperature (those should be the arguments to your function). Declare any necessary constants as constants*, not variables.

a) Calculate and plot the speed probability distribution functions for ^{4}He, ^{20}Ne, ^{40}Ar, and ^{132}Xe at 298.15 K (check your work against the plot on the Wikipedia page for the Maxwell-Boltzmann Distribution). Paste this graph in your notebook.

b) Calculate and append to the plot the speed probability distribution functions for ^{40}Ar at 200 and 400 K. Paste this graph in your notebook.

c) Is there a temperature at which the speed probability distribution function of ^{40}Ar is similar to the speed probability distribution function for ^{20}Ne at 298.15K? Append this to your plot. Comment in your notebook about the possibility, and support your argument with a graph or two. (You don't have to find an analytical solution; trial-and-error by graph is fine.)

- You may make the plots for this question from the command line or pull-down menus; they do not need to be generated/changed by a function.
- Make good plots! Consider the following points:

    1. Include axis labels (including units).
    2. Make the trace appearances have something to do with the data. Group "like" traces by using the same color, line style, etc.
    3. Include a legend, and put the items in a "good" order and with good names.

* Constants are a little like variables, but their value cannot be changed within a function. These are always hard-coded values. So you should use them only for things that really *are* constant. Good programming conventions are to

- use them for true, physical constants (like pi (already built in), conversion factors between Joules and calories, etc.)
- put them at the top of your procedure file, before the functions (all of the functions in your experiment will be able to use them)
- give them names in all capital letters, like JOULES2CALS, and use the all-caps version in your function (even though Igor wouldn't care)
- include units in their name if appropriate

In code, the JOULES2CALS constant might look like

```
constant JOULES2CALS = 1/4.184  // 1 J = 4.184 cal
```