CS 4630/5630 Kresman Homework 2 short

(Recap) In a chemical reaction, one or more substances transform to new substances as described by a chemical equation that gives the identities and quantities of the reactants and the products. Stoichiometry is all about such equations and is a foundational knowledge unit in the physical sciences (chemistry/chemical engineering).

As a new computational sciences intern working with chemists, you are put to work on Day 1 so the manager can get an idea of your comfort level with Chemistry and ability to work with physical scientists.

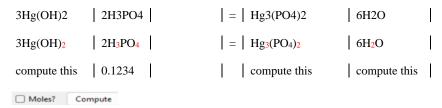
Problem 1: develop a (python) GUI stoichiometry app that takes in a balanced chemical equation and weight of a substance, and outputs some property of other substance(s). Read the balanced equation from an input file, Homework 2 short sample input.txt (just one line).

Interface:

- 3 rows of 6 column cells (text boxes): populate the corresponding cells of 1st row from the input file.
- 2nd row is transformed* values of 1st row (see Notes)
- One of the corresponding cells in the 3rd row is input lab measurement of that substance (in grams).
- A *checkbox* to specify the unit for *all* outputs checked means mole, else grams.

User inputs the lab measurement, checks/unchecks the checkbox and hits *Compute* button. The app computes/populates the other cells of the 3rd row. Assume valid input (no illegal compounds, etc.)

Sample run with checkbox unchecked. The app populates 1st two rows and computes 3rd row cells 1, 4, 5.



Problem 2 CS 5630 ONLY: Identify the limiting reagent, and theoretical yield of the (product) compounds in grams. Input is lab measurement, in grams, for all reactants. Tweak Problem 1 GUI, so one app does both problems! You can figure the limiting reagent (the one that is used up 100%) based on the class cookie discussion

Bonus credit, 5 points (CS 4630 ONLY): Do Problem 2 as well; bonus credit kicks in provided Problem 1 & 2 are BOTH 100% correct, else no bonus credit.

Notes:

- transformed*: 2nd row identical to 1st row except that the atom count shows up as a subscript
- My helper module, Chemistry.py (do NOT modify this file): Must use the functions noted below:
 - molesAndCompounds (compound) returns a list with two items: # moles and the compound
 - o example: molesAndCompounds ('Fe(OH)3') returns [1, Fe(OH)3]
 - atomCount (compound) returns a dictionary key is atom, and value is # atoms.
 - o example: atomCount ('Fe(OH)3') returns {'H': 3, 'Fe': 1, 'O': 3}
 - splitOnAtomCount (compound) returns a list in order of appearance: stuff, atom count, etc.
 - $\circ \quad \text{ example: splitOnAtomCount ('Hg3(PO4)2') returns ['Hg', '3', '(PO', '4', ')', '2']} \\$
 - numberAsSubscript ("123") returns 123 as a subscript.
 - o example: print ("hello" + numberAsSubscript ("123") + "World") prints hello₁₂₃World
 - symbolAndMassses (peirodicTableFileName) returns a dictionary key is atom, and value is mass, for all elements in the file.
 - o example: symbolAndMassses ('PeriodicTableData.xlsx') returns {'H': '1.008', 'He': '4.003' ...}
- PeriodicTableData.xls: Excel file of periodic table
- Homework 2 short sample input.txt: sample file to try out though the app should work with any valid input. The balanced equation in the file can have (up to) 3 reactants and (up to) 3 products.
- String tokenizer: "abc * 123 -456 * xyz".split ('*') returns ['abc ', '123 -456 ', 'xyz']. Works like a C++ tokenizer. (Delimiter in this example is *.)
- Use only the concepts we covered through Unit 6.

Canvas turn-in: lastnameHW2short.ipynb

Grading Rubric
_/7 Correct output _/5 Respects all items in 'Notes' above _/3 Interface