CS 4630/5630 Kresman Homework 3

**Problem 1** CS 4630 ONLY

Your manager is impressed with your on-time delivery of the stoichiometry app (that was assigned on Day 1), and your ability to interact with chemists! Sure enough, there is more workload in the pipeline. Recall that stoichiometry begins with balancing chemical equations, and that is what the manager wants you to handle next. Homework 2 is the front-end of the app, while the instant workload is the backend; however, both apps are distinct/disjoint.

(unbalanced) Chemical equations appear in an input file, one/line: compounds (or molecules) separated by a ‘+’ sign, while reactant and product separated by an ‘=’ sign - sample input/output below. [CS 4630: the app can be console or GUI-based, your call; as well, the app needs to work with just the 1st line in the file.]

(file input line) Hg(OH)2 + H3PO4 = Hg3(PO4)2 + H2O

(app output) 3Hg(OH)2 + 2 H3PO4 = 1Hg3(PO4)2 + 6H2O

**Problem 2** CS 5630 ONLY: Extend/integrate Homework 2 with Problem 1 above, i.e. add two additional buttons, *getFileName* & *getNextEquation*: click on getFileName to navigate to the file that has the chemical equations (so filename is not hardcoded); click on getNextEquation to read the next equation from the file, balance, and populate the 1st row (see Homework 2). Once 1st row is populated, all aspects of Homework 2 work as before.

**Resource/notes**:

* homework3SampeInput.txt: sample input file to try out, though the app should work with any valid input/file.
* Helper module, Helper2.py: Must use the function below:

atomCount (compound) returns a dictionary – key is atom, and value is # atoms.

* Example: atomCount (‘Fe(OH)3’) returns {'H': 3, 'Fe': 1, 'O': 3}
* Must use the sympy solver that we discussed.
* String tokenizer: “abc \* 123 -456 \* xyz”.split (‘\*’) returns ['abc ', ' 123 -456 ', ' xyz']. Works like a C++ tokenizer & delimiter in this example is \*.
* Like Homework 2, max 3 reactants and max 3 products. No error checking (assume valid input)

Bonus credit for CS 4630 ONLY: 3 points if the app loops through and balances correctly all equations in the file.

Use only the concepts we covered thus far. Canvas turn-in: lastnameHw3.ipynb, & a word doc with runs snapshots