CS 4630/5630 Kresman Homework 2

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).

**Problem 1**: As a new computational sciences’ intern working with chemists, you get to work on Day 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 substances.

Interface:

* 2 rows of 6 column input cells: 1st row is input of the balanced equation - (up to) 3 reactants and (up to) 3 products. [implied + sign b/w reactants, & between products]
* One of the corresponding cells in the 2nd row is also an input - lab measurement of that substance (in grams).
* A *checkbox* to specify the unit for *all* outputs – checked means molecules, else moles.

User inputs the equation, checks (or unchecks) the checkbox and hits *compute* button. The app computes/populates the other cells of the 2nd row. Assume valid inputs (no space or illegal compounds, etc.)

Sample run [eqn: 3Hg(OH)2 + 2H3PO4 = Hg3(PO4)2 + 6H2O] with checkbox unchecked - consider adding ‘=’ to separate reactants & products. The app computes output cells 1, 4, and 5.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| 3Hg(OH)2 | 2H3PO4 |  | = | Hg3(PO4)2 | 6H2O |  |
|  |  |  |  |  |  |  |
| compute this | 0.1234 |  |  | compute this | compute this |  |

How to compute? Use the skillset from Chemistry class/class discussion or Google; briefly, periodic table has atomic weight of 1 mole of an element in grams; to get weight of 1 mole of a compound, multiply the atomic weight of constituent element by the number of atoms of that element, and add them. If lab measurement notes a compound’s weight in grams, determine its weight in moles; then, use the molar ratio in the equation to find corresponding compound’s molar weight [for example, if 2nd compound’s lab measurement is 0.1234 grams, and corresponding moles is 0.456, then 1st compound is 3/2 \* .456 moles.

**Problem 2** CS 5250 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!]

**Resource/notes**:

* My helper module, Helper1.py: Has three functions that must be used:
* molesAndCompound (myCell) returns a list with two items: # moles and the compound
  + Example: molesAndCompound (‘Fe(OH)3’) returns [1, Fe(OH)3]
* atomCount (compound) returns a dictionary – key is atom, and value is # atoms.
  + Example: atomCount (‘Fe(OH)3’) returns {'H': 3, 'Fe': 1, 'O': 3}
* symbolAndMass (peirodicTableFileName) returns a dictionary – key is atom, and value is mass, for all elements in the file.
  + Example: symbolAndMass (‘PeriodicTableData.xlsx’) returns {'H': '1.008', 'He': '4.003' …}
* PeriodicTableData.xlsx: Excel file of periodic table

Use only the concepts we covered thus far. Canvas turn-in: lastnameHw2.ipynb, & a word doc with runs snapshots