

## 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 1<sup>st</sup> row from the input file.
- 2<sup>nd</sup> row is **transformed\*** values of 1<sup>st</sup> row (see Notes)
- **One** of the corresponding cells in the 3<sup>rd</sup> 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 3<sup>rd</sup> row. Assume valid input (no illegal compounds, etc.)

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

3Hg(OH) <sub>2</sub>	2H <sub>3</sub> PO <sub>4</sub>		=	Hg <sub>3</sub> (PO <sub>4</sub> ) <sub>2</sub>	6H <sub>2</sub> O	
3Hg(OH) <sub>2</sub>	2H <sub>3</sub> PO <sub>4</sub>		=	Hg <sub>3</sub> (PO <sub>4</sub> ) <sub>2</sub>	6H <sub>2</sub> O	
compute this	0.1234			compute this	compute this	

☐ Moles?

**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\***: 2<sup>nd</sup> row identical to 1<sup>st</sup> 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
    - example: molesAndCompounds ('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}
  - splitOnAtomCount (compound) returns a list in order of appearance: stuff, atom count, etc.
    - example: splitOnAtomCount ('Hg3(PO4)2') returns ['Hg', '3', '(PO', '4', ')', '2']
  - numberAsSubscript ("123") returns 123 as a subscript.
    - example: print ("hello" + numberAsSubscript ("123") + "World") prints hello<sub>123</sub>World
  - symbolAndMasses (periodicTableFileName) returns a dictionary – key is atom, and value is mass, for all elements in the file.
    - example: symbolAndMasses ('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