

Assignment #6

A **mole** is that quantity of a substance which contains 6.02×10^{23} particles. This number is called **Avogadro's number**. The quantity of any element or compound having a weight in grams equal to its atomic weight contains a mole of atoms or molecules respectively. Thus 1.008 grams of hydrogen contains 6.02×10^{23} atoms (the atomic weight of H is 1.0080), and 18.0154 grams of water contains 6.02×10^{23} molecules of water (the molecular weight of H_2O is $1.0080 \times 2 + 15.9994 = 18.0154$).

Thus the number of particles of a substance may be calculated from its weight in grams by:

$$\begin{aligned} \text{NumberOfParticles} &= \text{NumberOfMoles} \times \text{Avogadro'sNumber} \\ &= \frac{\text{WeightInGrams}}{\text{NumberOfGrams / mole}} \times \text{Avogadro'sNumber} \end{aligned}$$

Example: How many carbon dioxide molecules are there in 0.00220 grams of CO_2 ?

$$\begin{aligned} \text{NumberOfGrams / mole } CO_2 &= 12.011 + 15.9994 \times 2 \\ &= 44.0098 \text{ g / mole } CO_2 \end{aligned}$$

$$\begin{aligned} \text{NumberOfParticles} &= \frac{0.00220 \text{ g } CO_2}{44.0098 \text{ g / mole } CO_2} \times 6.02 \times 10^{23} \text{ particles / mole} \\ &= 3.01 \times 10^{19} \text{ particles} \end{aligned}$$

Write a program that will calculate the number of molecules of a substance given its weight in grams and its molecular formula. Assume an unsorted file *periodicTable.dat* that contains the atomic symbol, atomic number and mass number of several common elements. For example the data file may contain the following lines:

H	1	1.0080
He	2	4.00260
C	6	12.011
N	7	14.0067
Na	11	22.9898
....		

Create the file *periodicTable.dat* with a minimum of 25 elements.

Your program should ask the user to input the substance's molecular formula and weight and print the number of molecules. A typical dialogue would be:

Enter the molecular formula: CO2

Enter the weight in grams: 0.00220

The number of molecules in 0.00220 grams of CO2 is 3.01E19.

Enter the molecular formula: Fe2O3

....

Try your program on the following problems:

H2	5 grams
H2O	2.5 grams
Fe2O3	1 gram
C6H12O6	25 grams

Make up several more of your own. Be sure your program is clearly documented, structured, and uses meaningful variables. Output is to be both to a file as well as to the console. Turn in your program as well as input and output files.

Strategy

1. Create a function *readPeriodicTable* that reads the information in the *periodicTable.dat* file into three arrays: *atomicSymbol*, *atomicNumber*, *atomicMass*. Your function should also return the number of elements in the arrays.
2. Create a function *bubbleSort* that sorts the three arrays alphabetically.
3. Create a function *printTable* that prints a neatly formatted table of the information that you have sorted.
4. The *main* function should prompt the user for the molecular formula and the weight in grams.
5. The *main* function should call a function *numberOfGramsPerMole* which is given the molecular formula as a parameter (string) and returns the number of grams per mole. This function will have to parse the input string in order to separate each element and the number of atoms of that element. Note the following rules:
 - a. An element always begins with a capital letter and may be followed by a single lower case letter.
 - b. The absence of a number indicates a single atom of that element.

After determining the identity of the element and the number of atoms of that element the function calls another function, *findMassNumber* in order to determine the mass number of that element.

numberOfGramsPerMole then calculates, and eventually returns, the total number of grams per mole represented by that formula.

6. The function *findMassNumber* receives a symbol of an element as a parameter and returns its atomic mass by searching the arrays you created in steps 1 and 2. If the element is not in the table, it should print an error message and return a value which will allow the program to abort.
7. The *main* function then calls a function *calculateNumberOfParticles* that accepts the weight in grams and the number of grams per mole as parameters and returns the number of particles which is then printed by the *main* function.
8. The main function should repeat the process until the user indicates that there is no more data to be processed.