**Recitation 2**

**Topics**

* Functions
* Vectors

**Recitation Project**

We have been given a file of various molecules, specifically hydrocarbons. Hydrocarbons consist of only hydrogen and carbon atoms.

Each line of the file contains the name of the chemical followed by its molecular formula which will be in the form**:**C#H#, where # is the number of carbon (C) and hydrogen (H) atoms. (No name in the file contains blanks.)  An example is:

n-Butane C4H10

Note that it is possible for two different molecules to have the same formula. This won't effect our programming task, but don't be surprised if you see such examples in the sample input file.

It makes sense that if we want to do anything with these chemicals, we will want to keep all the information for each chemical, such as n-butane, together in a single "object". For this recitation, we will use a vector for that.

Using a vector to hold these two pieces of information for each molecule is certainly *not* the best choice. It would be better to either use something like C++'s pair which *can* only hold two items. Or even better, to define a *type* for this purpose. But we don't know how to define types yet and there's no overwhelming reason to make you learn about pairs here. So, a vector of vectors will be the easiest for us to work with.

So, for each of the molecules in the file, we will create a vector that holds the name and the formula.

What will we do?

* Open the file. To exercise our function writing skills, we will define a function that is passed an input file stream and uses it to open a file. Of course, this function will check that we succeed in opening the file. If we don't, it should display an appropriate error message and terminate the program.
  + How do you terminate a program?  Call the function exit, that takes a small non-negative integer as its only argument. You can choose whatever integer you like.
* Read the file of these moleclues. Fill a vector with all the information for all of the molecules. That means our vector of molecules will have to hold vectors that hold the two pieces of information about each molecule!
  + Again, write a function to do this.
  + What should the function get passed? We will pass it the the stream to read from and the vector to fill.
* Afterwards, we want to do some processing on this collection.  To keep the exercise short, we will just print them all out.
  + Actually, we will print them twice.  First we will print them all using an index variable for the vector and then print them all again using the ranged for
  + Each time, first print the formula and then print the name.

**Vector of vectors?**

How do we define a variable that holds a vector of vectors?

* Remember how to define a vector?
  + vector<int> vi; // a vector of integers
  + vector<double> vd; // a vector of doubles
  + vector<string> vs; // a vector of string
  + vector<*SomeType*> vS; // a vector of SomeType
* So to define a vector of vectors, we just have to put the *kind of vector* it is, where SomeType went. In our case it will be a vector of strings. (Remember, it will be holding the name and formula of the molecule.)
  + vector<vector<string>> vvs; // a vector that holds vectors of strings
    - Before C++11 we would have had to put a space between the two "right-angle-brackets".
* How about accessing an item in this vector of vectors of strings? If we think about the first item in that vector vvs, vvs[0], what sort of thing does it hold? A vector, certainly. If we have written out program correctly then it would be a vector of two items. The first we could refer to as vvs[0][0] and the second as vvs[0][1].

**An example**

Suppose this is the file:

Pentane C5H12

n-Butane C4H10

Propyne C3H3

Your program should store these in a vectorof vectors of strings. It will then display them as:

C5H12 Pentane

C4H10 n-Butane

C3H3 Propyne

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C5H12 Pentane

C4H10 n-Butane

C3H3 Propyne

See the attachments for an input test file.

#### Additional resources for assignment

* ile attachment [chemicals.txt](https://newclasses.nyu.edu/access/content/attachment/d5110493-7072-4a26-b7c9-8e41d1b52934/Assignments/7ac2bc71-c34d-48b1-a18c-a12d47c3e799/chemicals.txt) ( 1 KB; Sep 7, 2015 5:52 pm )

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