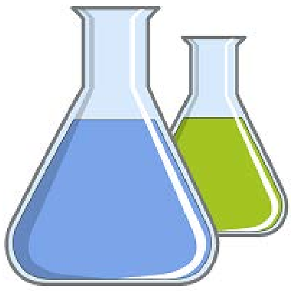


The Mad Chemist

Computer scientists are often called upon to write tools or process data for scientific and business applications. The project is often a model/simulation or a lookup tool. In this case, we have a chemist friend who is going mad from having to calculate the weights of molecules by hand. Our job is to write a tool that will parse a chemical formula and calculate the weight of the molecule. Maybe there's still time to keep our friend sane! This project will help you learn and practice:

- Creating projects with MS Visual Studio
- Designing and implementing software
- Practicing with C# syntax
- Debugging programs
- Simple search algorithms
- Parsing encoded strings
- Reading and writing text files
- Recursion (Apprentice-Level)

Program Description:

You are writing a program that calculates the atomic weight of simple molecules. The user will provide a chemical formula like "NaCl" as a command line parameter. Your program must calculate the weight of the molecule based on the weights of the individual atoms, which you can find in the periodic table. The periodic table will be provided as a text file.

In order to calculate the weight of the molecule, you must parse the molecular formula by breaking it apart into individual atoms. You can then lookup the weight of each atom in the periodic table and use the information to calculate the weight of the entire molecule.

Simple molecules are specified by listing each atom using its periodic symbol followed by a number, which indicates the count of that particular atom symbol (keep in mind that upper- and lower-case letters are important for element symbols). If no number is specified, it means there is only one of that type of atom. For example, H2O means that there are two atoms of hydrogen and one atom of oxygen. NaCl would be interpreted as one atom of sodium and one atom of chlorine.

*Note: The US National Institute of Standards and Technology has a publicly accessible database that may help you verify the accuracy of your work. The NIST Chemistry WebBook that allows you to lookup molecule names by formula, by name, and by weight.

Apprentice-Level (+1 honor, glory, and bragging rights):

To reach Apprentice-Level, your program should accept groups of atoms as part of the chemical formula. These groups are enclosed by parentheses and might be followed by a number, which tells how many of these groups are part of the molecule. For example, B(OH)3 contains one atom of boron and three atoms each of oxygen and hydrogen.

Professional-Level (+1 point extra credit):

Add an optional, second command line parameter to your program that takes the name of the molecule in addition to the atomic formula. Save the name of the molecule in a text file along with the atomic formula and molecular weight.

Your text file will start empty but will grow with time as you look up more and more molecules. When your program first runs, rather than immediately calculating the weight of the chemical formula, it should first check to see if the value is in the text file. If the molecule is already in your text file, there is no reason to read the periodic table file or to perform the weight calculation.

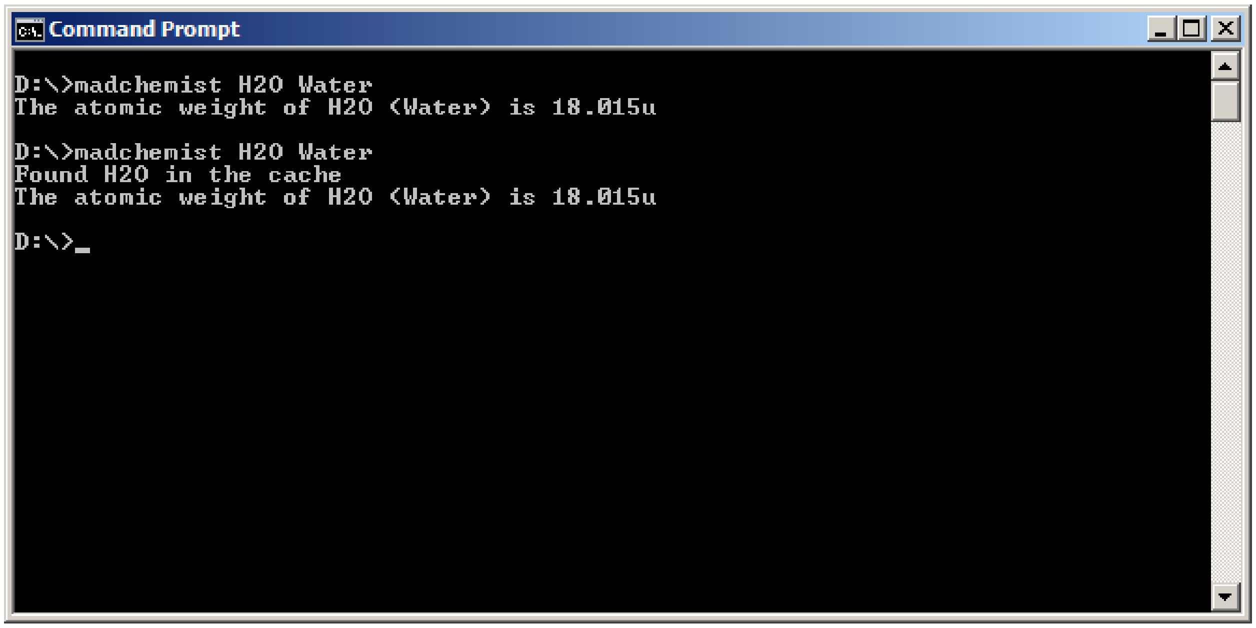
Allow the user to ask for the weight of a molecule by its name, and not just by its chemical formula. So now your program accepts either one or two parameters. If there are two parameters, they should be the atomic formula and the molecule name. If there is only one formula, the parameter could either be a molecule name or its atomic formula. You will need to include some logic to handle this ambiguity.

If the user specifies a molecule name and it is not already in your text file, you can report an error.

L33t Hacker-Level (+1 point extra credit):

Allow the user to input an atomic weight. Your program should read your text file and report the three known molecules whose weight most closely matches the input. If your text file is relatively small, this feature will be wildly inaccurate. But as you lookup more molecules, the accuracy will improve.

Example Output



```
D:\>madchemist H2O Water
The atomic weight of H2O (Water) is 18.015u

D:\>madchemist H2O Water
Found H2O in the cache
The atomic weight of H2O (Water) is 18.015u

D:\>_
```

Programming Style:

This course does not have a required coding style (at least not yet). Your code should be nicely arranged with proper whitespace, along with appropriate and consistently named variables/functions. Any code that is executed repeatedly should be put into its own function. This makes it easier for you and others to maintain the code.

Homework Submissions:

Please upload your source code to Blackboard. There should only be a single .cs file for this project. You'll find the upload page by clicking "Project #2: The Mad Scientist" on the Assignments page. I will cut-and-paste your code into a scratch project in order to review it, compile it, and test it.

Class Presentations:

You will need to present your code to the class. You must talk through the most challenging part of the project: show this portion of your code, explain the problem you encountered and how you went about solving it. You will only have 2-3 minutes to demonstrate which is NOT MUCH TIME.