CSCI 111 Data Types Assignment

Aim:
To write a C++ program involving arrays, structs file I/0 and files.

Procedure:
Write a program to read in a string of up to 30 characters. These input strings should reside in an input text file of your own making.
Each string will represent a chemical compound.
For example, water (H2O) would be input as H2O; sulphuric acid (H2SO4), salt (NaCl) would be just that. Note that some compounds have the same symbol more than once - ethanol, for instance is C2H5OH.

Write a function which, when passed the string from A, returns an array of pairs, each pair containing the chemical element + the number of atoms.
Thus, H2O would return:
H, 2 atoms
O, 1 atom;
NaCl would return
Na, 1 atom
Cl, 1 atom;
C2H5OH returns
C, 2 atoms
H, 6 atoms
O, 1 atom.
How do we return pairs from a function? By creating an array, where each element is a struct consisting of a string to contain the symbol, and a short integer to contain the number of atoms. The function must be capable of handling compounds with more than 9 atoms of an element such as naphthalene - C10H8.

Test your function by trying assorted compounds (periodic table provided in the file "period.tbl"), printing out the elements and the number of atoms of each, plus the total number of atoms in the compound.

On the server you will find a text file called "period.tbl". This file contains a list of the first (?) elements of the periodic table listing

Symbol	Name	Atomic_number	Atomic_weight
Ag	Silver	47	107.87
F	Fluorine	9	19.00

Write a function which opens the file and reads the contents of the file into a suitable array of structs to store the information. Assume that the names are no longer than 14 characters, and that the file contains no more than 110 elements. The array of structs should be global to all the functions in this program, but not available to the main program. The elements are in order of atomic number, starting with hydrogen, atomic number 1.

Write a function which, when passed a string containing a symbol, returns the name, atomic number and atomic weight for the element in the periodic table. This requires a linear search of the array containing this information, looking for the correct symbol. The atomic number can be returned as the value of the function, with a return value of 0 indicating that the symbol could not be found in the table.

Finally, write a function which, when passed the array definition of a compound, prints out the number of atoms of each element by full name and symbol, and totals the required multiples of each atomic weight to yield (an estimate of) the molecular weight. It should also sum the atomic numbers to produce the number of protons present in the

molecule. (Apologies to any chemists who are offended by such simplifications.)

Improve the speed of the search of the periodic table by using, for example, some form of sorting of the information, and perhaps some more efficient search procedure.

Submission:
The following C++ files:
A main.cpp file, which should repeatedly read a compound, reporting the information in Band E, until an end-of-file is detected;
A ???.cpp file, with a suitable name, of your own choosing, containing the periodic table array and all functions.
A ???.h header file, again with a suitable name of your own choosing, containing prototypes of the functions callable from the user program.
You should ensure that the file names are all lower case, and that the header file, when included in your files, has the same case.