Tecnológico de Monterrey
campus Querétaro

Computational Thinking for Engineering (Gpo 416)

Evidence 2. Final code delivery

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This program allows you to input the name of a compound and it will tell you its molecular geometry, bond angle and useful information about elements such as Element Symbol, Atomic Number, Valance electrons, Full shell, Electron Configuration and Noble Gas Configuration.

This project was inspired by a chemistry class where once again I was faced with a bit of a tedious task, finding the Molecular Geometry of compounds. This is a fairly simple thing to do, but it gets old quite quick when every exercise starts with defining it. Also, it's just time consuming and boring when you already know exactly how to do it. So, to make the process of finding these geometry´s more efficient, this program was created.

It´s divided in 4 functions, the first three functions allow the user to find a compounds Molecular Geometry. To do this the function 1. Total Bonds is called to calculate the amount of bonds found in the compound. Then the function 2. Lone Pairs is called to, in case there is a central atom, find how many unbonded electrons or lone pairs it has. Lastly the function 3. Molecular Geometry and Bond Angle is called to analyze through the set of data, found in MolecularG.txt, to determine which condition is met by the compound and determine its Molecular Geometry and bond angle.

A fourth function was created to encapsulate useful information about the elements included in this first version of the program. These elements are, Hydrogen, Helium, Lithium, Beryllium, Boron, Carbon, Nitrogen, Oxygen, Fluorine and Neon.

The program has certain limitations as to what compounds molecular geometry it can determine. This is due to the fact that the databases cover until the tenth element of the periodic table. Also, this first version of the program is unable to analyze compounds with double or triple bonds correctly. There are multiple areas of opportunity for the next version, apart from the two already mentioned, some other areas of improvement are, the amount of inputs the user must write and further functions should be added to allow the user to obtain more information about the element or compound they wish to analyze.

How should the user execute the program?

Once the program is run, the user can pick between finding the molecular geometry of a compound or attain general information of an element.

To attain the general information of an element it is very straight forward as all the user has to do, is input the number that corresponds to this function and the element he or she wishes to analyze.

In case the user wants to calculate the molecular geometry of a compound, he or she must select the function that corresponds to the first step, in this case "1. Total Bonds". Once this function is completed the user will once again be presented with the menu. The user must now choose the second step of the process "2. Lone Pairs",

this is also indicated as the program is run, as to guide the user through the program. Lastly the last step must be chosen “3. Molecular Geometry and Bond Angle” to attain the last result.

Apart from these two functions there is one more called “5. Exit” to allow the user to exit the program by being kindly said “Goodbye”.

The test cases chosen to allow for the different molecular geometries to be displayed are the following:

H2: Linear, 180°

BeF2: Linear, 180°

H2O: Bent, less than 109.5°

BF3: Triagonal Planar, 120°

NH2F: Triagonal Pyramidal, less than 109.5°

CH4: Tetrahedral, 109.5°

On the left are the compounds than need to be given by the user following the programs directions and on the right are the final expected outputs.

To analyze more exactly how every function works and how the program runs, be sure to check out the file: “Code with Test Cases and Comments”.