Bond Length and Angle Instructions

Installation

Open Babel

For Linux users (e.g. Ubuntu), download Open Babel via the command line (e.g. sudo apt install openbabel).

For Windows users, download the latest release from here: https://github.com/openbabel/openbabel/releases/tag/openbabel-3-1-1. Choose to download "OpenBabel-3.1.1-x64.exe" if you have a 64-bit operating system (you probably do).

Python 3

You need to have Python 3 for any of this to work.

xyz2Tab

Go to https://github.com/AkiraY1/StudentsOnTheBeamline/blob/main/xyz2tab_mod.py. Click on "Code" and click "Download ZIP". Unzip the folder and delete everything in the folder, except for "xyz2tab_mod.py".

Usage

Put all of your PDB files into the same folder as "xyz2tab_mod.py".

Open up a terminal session. Make sure you're in the same folder as the PDB files. Then enter the following (write your own filenames):

    obabel filename.pdb -O outputfilename.xyz

Now, you have the xyz file for one of your pdb files! Woohoo! Make sure you're in the same folder as the xyz file and "xyz2tab.py". **Change line 23 of xyz2tab_mod.py every time you run xyz2tab_mod.py to reflect the name of the output CSV file.** Now, type the following to run xyz2tab.py (obviously write your own filename):

    python xyz2tab_mod.py filename.xyz

DO NOT open the Excel file (the one that ends with .csv) before xyz2tab.py is done running.

Formatting the Excel File

Hyphens

Once you open the Excel file, you will realize that all the hyphens ("-") have been replaced by " â€" ". To replace all these in the file at once, click Control-f (for Windows) or Command-f (for Mac OS). Go to the "replace" tab. Copy the following into the "Find what" field:

    â€"

Under "Replace with", copy the following:

    -

Finally, click "Replace all". You can close the tab once Excel confirms it has made all the replacements.

NOTE 1

Technically, the output is not an Excel file format, it's a CSV file, but it's easier to just call it an Excel file to not confuse people.

NOTE 2

Since all the data is added on top of each other in the Excel file, you will have to scroll down to find each table manually. There is an empty row between each table in the Excel file.