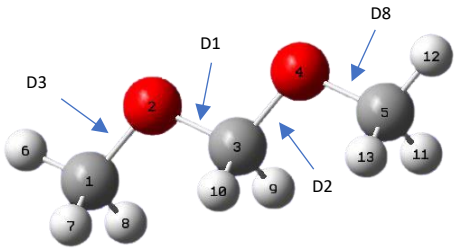
Rotor Scan Input Python Script Tutorial

Motivation: Typically, to run a Gaussian scan job, you must identify a dihedral of interest on a z-matrix-format input file (.gjf) and write *s 36 10.0* next to it (in addition to changing the route section with the appropriate directions). This can be time-consuming if working with multiple files and increases the likelihood of making a silly mistake somewhere. The goal of these scripts is to identify and generate input (.gjf) files for every rotor of a given molecule (on z-matrix format). It works as well for multiple molecules at the same time.

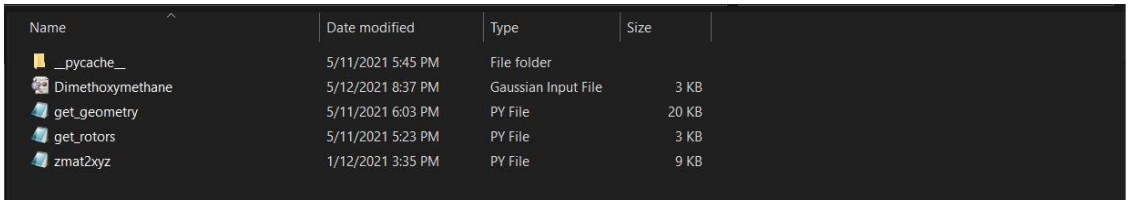
There are 3 scripts that you will be using for this:

- get_rotors.py
- zmat2xyz.py
- get_geometry.py

Step 1: Place all 3 .py scripts in the same directory as the molecule you want to generate input files for. For this demo, we will be using Dimethoxymethane.

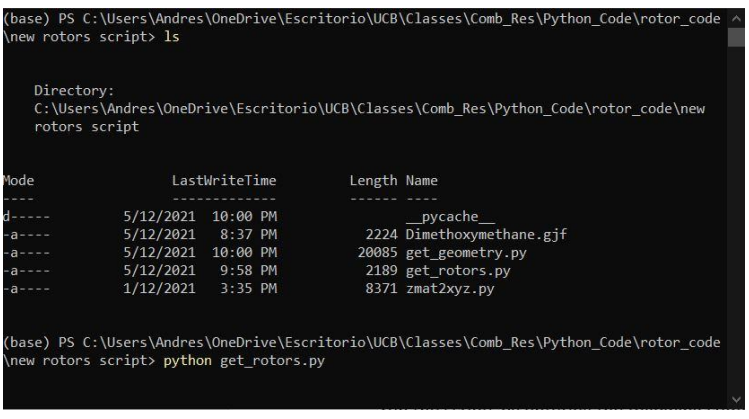


Dimethoxymethane: Has 4 rotors. For the numbering above, they will correspond to D3, D1, D2 and D8.



Name	Date modified	Type	Size
__pycache__	5/11/2021 5:45 PM	File folder	
Dimethoxymethane	5/12/2021 8:37 PM	Gaussian Input File	3 KB
get_geometry	5/11/2021 6:03 PM	PY File	20 KB
get_rotors	5/11/2021 5:23 PM	PY File	3 KB
zmat2xyz	1/12/2021 3:35 PM	PY File	9 KB

Step 2: Navigate to this directory in your terminal (make sure you have python 3 installed), and run the scripts by entering the following command *python get_rotors.py*



```
(base) PS C:\Users\Andres\OneDrive\Escritorio\UCB\Classes\Comb_Res\Python_Code\rotor_code
\new rotors script> ls


    Directory:
    C:\Users\Andres\OneDrive\Escritorio\UCB\Classes\Comb_Res\Python_Code\rotor_code\new
    rotors script


Mode                 LastWriteTime         Length Name
----                 -------------         ------ ----
d-----         5/12/2021  10:00 PM                __pycache__
-a----         5/12/2021   8:37 PM           2224 Dimethoxymethane.gjf
-a----         5/12/2021  10:00 PM          20085 get_geometry.py
-a----         5/12/2021   9:58 PM           2189 get_rotors.py
-a----         1/12/2021   3:35 PM           8371 zmat2xyz.py


(base) PS C:\Users\Andres\OneDrive\Escritorio\UCB\Classes\Comb_Res\Python_Code\rotor_code
\new rotors script> python get_rotors.py
```

Step 3: Specify if the file/molecule in question is a Transition State or not (y/n)

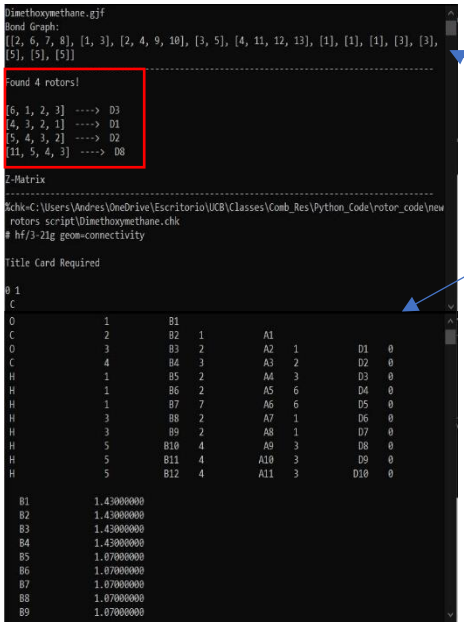
```
(base) PS C:\Users\Andres\OneDrive\Escritorio\UCB\Classes\Comb_Res\Python_Code\rotor_code
\new rotors script> ls


    Directory:
    C:\Users\Andres\OneDrive\Escritorio\UCB\Classes\Comb_Res\Python_Code\rotor_code\new
    rotors script


Mode                 LastWriteTime         Length Name
----                 -------------         ------ ----
d-----         5/12/2021  10:00 PM                __pycache__
-a----         5/12/2021   8:37 PM           2224 Dimethoxymethane.gjf
-a----         5/12/2021  10:00 PM          20085 get_geometry.py
-a----         5/12/2021   9:58 PM           2189 get_rotors.py
-a----         1/12/2021   3:35 PM           8371 zmat2xyz.py


(base) PS C:\Users\Andres\OneDrive\Escritorio\UCB\Classes\Comb_Res\Python_Code\rotor_code
\new rotors script> python get_rotors.py
Is Dimethoxymethane.gjf a TS? (y/n): n
```

Step 4: Specify how many procesors you want to allocate for all the rotor scans for that specific file/molecule.

```
(base) PS C:\Users\Andres\OneDrive\Escritorio\UCB\Classes\Comb_Res\Python_Code\rotor_code
\new rotors script> ls


    Directory:
    C:\Users\Andres\OneDrive\Escritorio\UCB\Classes\Comb_Res\Python_Code\rotor_code\new
    rotors script


Mode                 LastWriteTime         Length Name
----                 -------------         ------ ----
d-----         5/12/2021  10:00 PM                __pycache__
-a----         5/12/2021   8:37 PM           2224 Dimethoxymethane.gjf
-a----         5/12/2021  10:00 PM          20085 get_geometry.py
-a----         5/12/2021   9:58 PM           2189 get_rotors.py
-a----         1/12/2021   3:35 PM           8371 zmat2xyz.py


(base) PS C:\Users\Andres\OneDrive\Escritorio\UCB\Classes\Comb_Res\Python_Code\rotor_code
\new rotors script> python get_rotors.py
Is Dimethoxymethane.gjf a TS? (y/n): n
How many processors?10
```

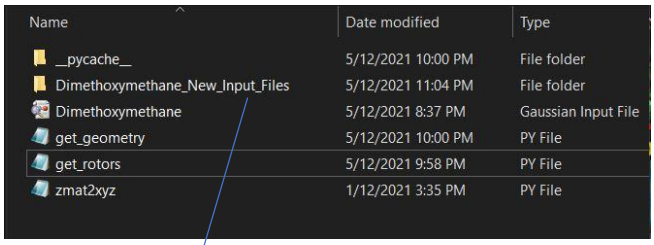
Step 5: Output!

Molecule's rotors

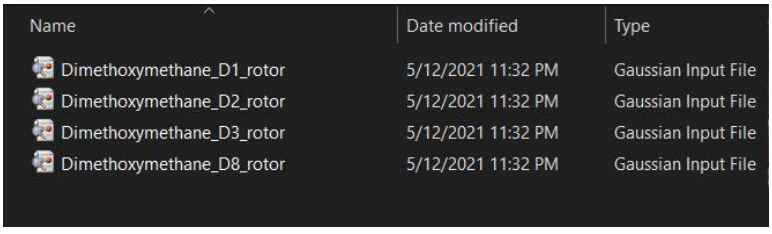


Molecule's bond

Molecule' z-matrix



Input files are inside newly created directory.



This process can be done with multiple files at a time, in which case multiple directories will be created with each molecules respective rotor input files inside each one.