

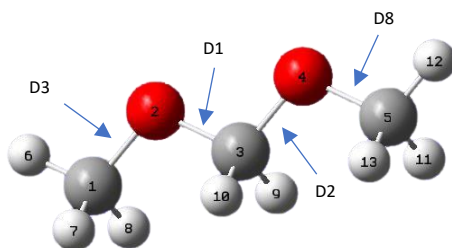
Rotor Scan Input Python Script Tutorial

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 processors 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!

```
Dimethoxymethane.gjf
Bond Graph:
[[2, 6, 7, 8], [1, 3], [2, 4, 9, 10], [3, 5], [4, 11, 12, 13], [1], [1], [1], [3], [3],
[5], [5], [5]]

Found 4 rotors!
[6, 1, 2, 3] ----> D3
[4, 3, 2, 1] ----> D1
[5, 4, 3, 2] ----> D2
[11, 5, 4, 3] ----> D8

Z-Matrix
-----
#chk=C:\Users\Andres\OneDrive\Escritorio\UCB\Classes\Comb_Res\Python_Code\rotor_code\new
rotors script\Dimethoxymethane.chk
# hf/3-2lg geom-connectivity

Title Card Required
B 1
C
C 1
C 2
D 3
C 4
H 1
H 1
H 3
H 3
H 5
H 5
H 5
B1 1.43000000
B2 1.43000000
B3 1.43000000
B4 1.43000000
B5 1.07000000
B6 1.07000000
B7 1.07000000
B8 1.07000000
B9 1.07000000
```

Molecule's rotors

Molecule's bond

Molecule' z-matrix

Name	Date modified	Type
pycache	5/12/2021 10:00 PM	File folder
Dimethoxymethane_New_Input_Files	5/12/2021 11:04 PM	File folder
Dimethoxymethane	5/12/2021 8:37 PM	Gaussian Input File
get_geometry	5/12/2021 10:00 PM	PY File
get_rotors	5/12/2021 9:58 PM	PY File
zmat2xyz	1/12/2021 3:35 PM	PY File

Input files are inside newly created directory.

Name	Date modified	Type
Dimethoxymethane_D1_rotor	5/12/2021 11:32 PM	Gaussian Input File
Dimethoxymethane_D2_rotor	5/12/2021 11:32 PM	Gaussian Input File
Dimethoxymethane_D3_rotor	5/12/2021 11:32 PM	Gaussian Input File
Dimethoxymethane_D8_rotor	5/12/2021 11:32 PM	Gaussian Input File

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.