ICSSgen

powerd by python

ICSSgen Manual

Input file generator for ICSS calculation

---------- Developed and Edited by ----------

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1. Overview

1.1 About ICSSgen

ICSSgen is an input file generator for ICSS (2D NICS) calculation. ICSSgen is open-source, free, high-efficient and user-friendly. ICSSgen supports macOS, Linux and Microsoft Windows operating systems. Source code of ICSSgen is also provided, thus, users can also run ICSSgen through Python IDE.

ICSSgen can be download at from author's website (https://www.wangzhe95.net/program) and author GitHub homepage (https://github.com/wongzit/ICSSgen).

1.2 How it Works

ICSSgen reads an input file including the target molecular coordinates, and adds ghost atom Bq to the end of the input file. User can define the plane, altitude, range and grid quality from ICSSgen.

2. Install/Run ICSSgen

2.1 Running with Source Code

If Python IDE is pre-installed in your computer, you can run ICSSgen with source code. Python 3.7 or newer is recommended. ICSSgen may not work normally with Python 2.

For Mac users who want to run ICSSgen with source code, please run following command in terminal:

```
python3 /path_to_ICSSgen/ICSSgen_v1_31_source.py
```

2.2 Running on macOS with Executable File

2.2.1 Use Packaged Executable File

The pre-packaged executable file is attached in the *packaged* folder. File "*ICSSgen_v1_31_catalina*" should be working normally on macOS 10.15 or newer, file "*ICSSgen_v1_31_m1*" should be working normally on Mac with Apple M1 chip. You can run ICSSgen by double click and ICSSgen will be running in terminal window.

2.2.2 Package Source Code into Executable File

If 2.2.1 is not work for some reason, you can try following steps to package ICSSgen by yourself.

1) Open terminal, execute `pip3 install pyinstaller` to install necessary packages.
2) Assume the source code file is located "*/home/user/ICSSgen/ICSSgen_v1_31_source.py*", execute command below.

   ```
   pyinstaller ICSSgen_v1_31_source.py --onefile
   ```

3) After that an executable file would be generated in *dist* folder. (Only executable file is needed, you can delete other files generated by pyinstaller.
4) Now you can run ICSSgen by double clicking.

2.3 Running on Linux with Executable File

1) Assume the executable file is located "*/home/user/ICSSgen/packaged/ICSSgen_v1_31_linux*", run below command to add executable permission to it.

   ```
   chmod +x /home/user/ICSSgen/packaged/ICSSgen_v1_31_linux
   ```

2) (Optional) Assume the shell is bash, add below lines to *~/.bashrc* file.

   ```
   alias icssgen=/home/user/ICSSgen/packaged/ICSSgen_v1_31_linux
   ```

3) After re-entering the terminal, and you can run ICSSgen at any dictionary by execute "`icssgen`" command. If you passed the step (2), you need to execute the full path to *ICSSgen_v1_31_linux* for running it.

2.4 Running on Microsoft Windows with Executable File

Find "*ICSSgen_v1_31_win.exe*" file in program folder, double click it and ICSSgen will be running in command line window.

3. How to Use

3.1 Before Running

You need prepare a Gaussian input file (*.gjf* or *.com*) including route section, and molecular coordinates. Please notice that only Cartesian coordinates is allowed. An example input file of benzene is attached in *example* folder:

```
%nprocshared=8
%mem=10GB
#p nmr=giao rb3lyp/6-31g(d)

Benzene_opt

0 1
 C              -1.33923600   -0.39585300    0.00000500
 C              -0.32668500   -1.35773000    0.00006900
 C               1.01242100   -0.96187800   -0.00005500
 C               1.33920200    0.39596500    0.00000800
 C               0.32679800    1.35770000    0.00006200
 C              -1.01250100    0.96179800   -0.00005800
 H              -2.38133000   -0.70401000   -0.00006600
 H              -0.58108600   -2.41424500    0.00007900
 H               1.80037500   -1.71023400   -0.00015400
 H               2.38136700    0.70385800    0.00000700
 H               0.58095200    2.41426700    0.00001800
 H              -1.80027600    1.71035300   -0.00006300
```

3.2 Generate ICSS Input

*In this section, user inputting is colored in red.

1) Run ICSSgen, the ICSSgen will request an (original) input file. You can drag the input file into the command window, or input the full path to the input file. Then, press enter to submit.

```
Please specify the original input file path:
(eg.: /ICSSgen/example/benzene.gjf)
/Users/path_to_ICSSgen/example/benzene.gjf
```

2) Specify the plane which ICSS map would be plot. The plane is defined in *XY*, *XZ* and *YZ* with no case-sensitivity. So, for user inputting, "xy", "XY" or "xY" are same.

```
Please specify the plane for ICSS map (XY, XZ, YZ):
xy
```

3) Specify the altitude over the molecular plane. The altitude is defined in Å.

```
Please input the altitude over the plane (in angstrom):
1
```

4) Specify the ICSS map range. For each direction, two numbers for minimum and maximum is needed. After finish, the program will print out the user-determined parameters.

```
Please specify the range of X axis (in angstrom, eg. -10 10):
-5 5

Please specify the range of Y axis (in angstrom, eg. -8 8):
-5.5 5.1

2D-ICSS(XY,1.0) map in [X: -5.0 to 5.0, Y: -5.5 to 5.1].
```

5) Specify the grid quality. The grid quality is defined by the distance between two neighboring ghost atoms. Smaller grid value will give a smoother ICSS map, but more calculation cost is necessary. In my experience, a grid value of 0.25 is enough to produce a perfect ICSS map. The default value of ICSSgen is 0.2, you can press enter directly to use 0.2.

```
Please specify the grid quality (value smaller than 0.25 is recommanded):
(press Enter to use default value 0.2)
0.25
ICSSgen will use grid quality of 0.25.
```

6) A new input file for ICSS calculation would be generated in the same dictionary as original input file, named with "*xxx_ICSS_plane_altitude.gjf*". ICSSgen termination.

3.3 After Running

Open the ICSS input file with text editor, and check whether syntax error. Then, submit it to Gaussian calculation.