ICSSgen v1.3.1

Input file generator for ICSS (2D-NICS) calculation.

Last update: 2021-04-22

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Update history

v1.3.1 (2021-04-22)

1. Executable program file updated, source code is provided.
2. Now a quote will be displayed before termination.
3. Document is updated.

v1.2.1 (2021-04-21)

1. Now executable file for all platform is available.
2. ~~Source code is deleted.~~

v1.2 (2021-04-20)

1. Now you can customize grid quality through program.
2. More stable input file reader was introduced.
3. Running on Linux platform was tested.

v1.1 (2021-04-20)

1. Program will not be terminated by error inputting when specify the map range.
3. Bug fix.

Platform

For all platform

Python code is provided, if your computer already installed with Python 3, you can run ICSSgen with:

```
python3 ICSSgen_v1_31_source.py
```

NOTICE: Python 3.7 or newer is recommended, ICSSgen may not work normally under Python 2.

For macOS

Executable file **ICSSgen_v1_31_catalina** has been tested on macOS Catalina 10.15.7 and Big Sur 11.2.3 on Mac with Intel-CPU. If you are using Mac with M1 chip, running ICSSgen with **ICSSgen_v1_31_m1** is recommended.

For Linux

Before running for the first time, you may need to add permission by:

```
chmod +x ./path_to_ICSSgen/ICSSgen_v1_31_linux
```

Add following command to environmental variables (for bash):

```
alias icssgen=./path_to_ICSS/ICSSgen_v1_31_linux
```

and you can run ICSSgen by `icssgen`.

For Microsoft Windows

Executable file **ICSSgen_v1_31_win.exe** has been tested on Windows 10 Education (x64) with Intel Core i7-10700. Double click to run it.

How to use

NOTICE: ICSSgen only generates input file for Gaussian. More details in program manual.

1. Prepare the input file including calculation route lines, title, charge and spin multiplicity, and Cartesian coordinate.

EXAMPLE: Input file of benzene on XY plane

```
%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
```

2. Run ICSSgen.

3. Drag the input file to the program, and press Enter.

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

4. Specify the plane for ICSS calculation, please input "xy", "xz" or "yz" (Not case-sensitive).

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

5. Specify the altitude for ICSS calculation, for on-plane calculation, please input 0. The value is in angstrom.

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

6. Range specification. Please input two numbers (float is okay) separated by space, eg. -10

10, the range will be set as [-10,10].

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

Please specify the range of Y axis (in angstrom, eg. -8 8):
(user input): -5.0 5.0
```

7. Grid quality: smaller value will give you a smoother ICSS map but more expensive calculation cost is needed. The default value is 0.2.

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

8. New input file named with **ICSS_plane_altitude.gjf** would be generated. You can submit this input file for Gaussian calculation. Enjoy!

Problem

1. ~~Once you get the input file for ICSS calculation, please open it by text editor before submit to Gaussian calculation. Sometimes the unnecessary line-break in original input file may be remain to the ICSS input file, these line-break will cause error during calculation.~~
   This problem has been fixed but I still recommand you to check the input file befor submitting to Gaussian.

   Unnecessary line-break

```
 H                  2.38136700    0.70385800    0.00000700
 H                  0.58095200    2.41426700    0.00001800
 H                 -1.80027600    1.71035300   -0.00006300
                                                          # <--- this is
unnecessary line-break
 Bq      -3.0      -3.0      1.0
 Bq      -3.0      -2.8      1.0
 Bq      -3.0      -2.6      1.0
```

No necessary line-break

```
 H                 2.38136700    0.70385800    0.00000700
 H                 0.58095200    2.41426700    0.00001800
 H                -1.80027600    1.71035300   -0.00006300 Bq      -3.0
-3.0      1.0     # <--- a line-break needed
 Bq      -3.0      -2.8      1.0
 Bq      -3.0      -2.6      1.0
```

From author

If you found any bugs, please contact me (wongzit@yahoo.co.jp).

More information about me, please check my personal website.

Hope you enjoy this program!