ICSSgen3D & ICSScub3D Manual

Python program kits for 3D-ICSS calculation

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

Zhe Wang

https://www.wangzhe95.net

Graduate School of Science

Hiroshima University, Hiroshima, Japan

E-mail: wongzit@yahoo.co.jp

[Website]

https://www.wangzhe95.net/program-icssgen3d

https://www.wangzhe95.net/program-icsscub3d

1. Overview

1.1 About

We already presented the ICSSgen and ICSScsv, two Python programs for 2D-ICSS calculation. Now, the 3D version is coming out. ICSSgen3D and ICSScub3D are open-source, free, high-efficient, and user-friendly. We provide the executable files for macOS/Linux and Microsoft Windows, and the source code

ICSSgen3D and ICSScub3D can be download at from author's website (https://www.wangzhe95.net/program) and author's GitHub homepage (https://github.com/wongzit).

1.2 How it Works

ICSSgen3D reads an original input file, and add ghost atoms to the end of the file. ICSScub3D can process the output files, extracting the magnetic shielding tensors and save them into a *.cub* file.

2. Install and Usage

2.1 Run with Source Code

If Python IDE is already installed in your computer, you can run the program with the source code. Python 3.9 is recommended. You can download the newest version of Python from its homepage (https://www.python.org).

For macOS and Linux users who want to run with source code, please run following command in terminal:

```
python3 /path_to_program/program_src.py
```

For Windows users, please execute following command in PowerShell or Command Prompt (*cmd.exe*):

```
py3 / path_to_program/program_src.py
```

2.2 Run with Executable File

All executable files (if available) are pre-packaged in *execufiles* folder.

For all platforms, users can run the program with the executable files by double click. For macOS/Linux users, you may need to add permission to the executable file before running for the first time. Assume the executable file is located at "*/home/user/program/execufiles/program_linux*", run below command to add executable permission to it.

```
chmod +x /home/user/program/execufiles/program_linux
```

If the pre-packaged executable files do not work normally, please try to run with source code, or package from source code with packaging tools like *pyinstaller*.

2.3 Common Issues

If the packaged programs cannot work due to system security problem, please refer to the "Mac/Windows Users Must Read" file for solution.

3. How to Use

In this section, user-inputted commands are colored in red.

3.1 Create 3D-ICSS Input Files with ICSSgen3D

1) Prepare an original input file before running ICSSgen3D. The input file should include the route line (*.chk* file path, calculation method, and geometric specification). An example is shown below:

```
%chk=methylazulene.chk
#p nmr=giao rb3lyp/6-31g(d)

optimized_1-methylazulene

0 1
 C                 -2.68122300   -0.69593600    0.00002600
 ...
```

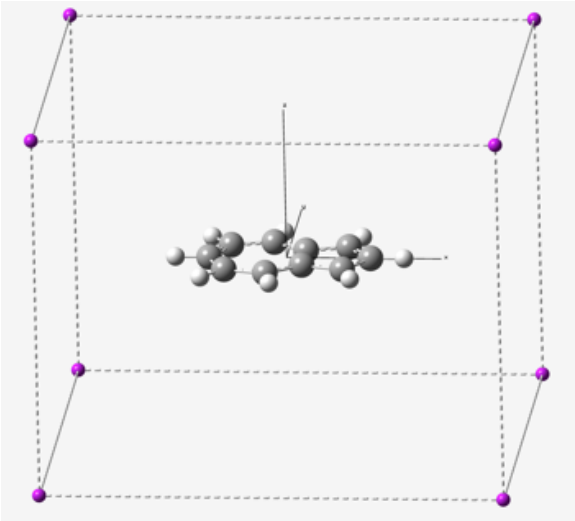
2) Run ICSSgen3D, the program will request the path for *Gaussian* input file. You can drag the input file into the command window or input the full path to it.

```
Please specify the original input file path:
(e.g.: /ICSSgen3D/example/methylazulene.gjf)
/Users/wangzhe/Desktop/methylazulene.gjf
```

3) Specify the calculation region. The region is defined in the range of X, Y, and Z axis.

```
Please specify the range of X axis (in angstrom, e.g., -10 10):
-7.5 7.5

Please specify the range of Y axis (in angstrom, e.g., -8 8):
-6.5 6.5

Please specify the range of Z axis (in angstrom, e.g., -8 8):
-6 6

3D-ICSS map in [X: -7.5 to 7.5, Y: -6.5 to 6.5, Z: -6.0 to 6.0].
```

In this example, the ghost atoms would be added in the cuboid, with X in [–7.5, 7.5], Y in [–6.5, 6.5] and Z in [–6, 6], as shown in the following figure.



4) Specify the grid quality of 3D-ICSS calculation. The default grid value is 0.25, you can press ENTER key to use the default value.

```
Please specify the grid quality:
(press Enter to use default value 0.25)
(ENTER)
ICSSgen3D will use grid quality of 0.25.
```

5) The ICSSgen3D will create several input files for ICSS calculations, name as "*xxx_3DICSS_0001.gjf*", "*xxx_3DICSS_0002.gjf*", "*xxx_3DICSS_0003.gjf*", ... Maximum Bq atom number is 7000 in one file.

```
/Users/tetsu/Desktop/methylazulene_3DICSS_0001.gjf has been saved.
/Users/tetsu/Desktop/methylazulene_3DICSS_0002.gjf has been saved.
/Users/tetsu/Desktop/methylazulene_3DICSS_0003.gjf has been saved.
…
*********************************************************************************

                Input files are successfully generated.
              Please submit these input files to Gaussian,
                  and save the output as .log files.

                   Normal termination of ICSSgen3D.

*********************************************************************************
```

6) Please submit these input files to *Gaussian* calculation. If you are using Bash Shell on your *Gaussian* machine, you can try author's RunGJF (https://github.com/wongzit/minorScripts), a Bash Shell script for submitting *Gaussian* jobs automatically.

3.2 Usage of RunGJF

1) Copy the RunGJF.sh to your calculation folder including all "*xxx_ 3DICSS_ 0001.gjf*", "*xxx_ 3DICSS_ 0002.gjf*", "*xxx_ 3DICSS_ 0003.gjf*", ... files.

2) Add permission to RunGJF.sh, and execute it:

```
chmod +x /path_to_RunGJF/RunGJF.sh
/path_to_RunGJF/RunGJF.sh
```

RunGJF will run all *.gjf* files in current dictionary.

3.3 Process 3D-ICSS Output with ICSScub3D

1) Run ICSScub3D.

2) Specify the path to output files. If you input *.../path/azulene_ 3DICSS_*, the output files *.../path/azulene_ 3DICSS_ 0001.log*, *.../path/azulene_ 3DICSS_ 0002.log*, *.../path/azulene_ 3DICSS_ 0003.log*, ... will be loaded to ICSScub3D. So, don't include the file number and "*.log*" in the path.

```
Please specify the Gaussian output file path of NMR task:
Assume that you input "/path/ben_", then /path/ben_0001.log, /path/ben_0002.log
/path/ben_0003.log, ... will be loaded.
(e.g.: /ICSScub3D/example/methylazulene_3DICSS_)
/Users/wangzhe/Desktop/example/methylazulene_3DICSS_
```

3) The ICSScub3D will load all of the output files in the inputted dictionary, it may take some time to load all files.

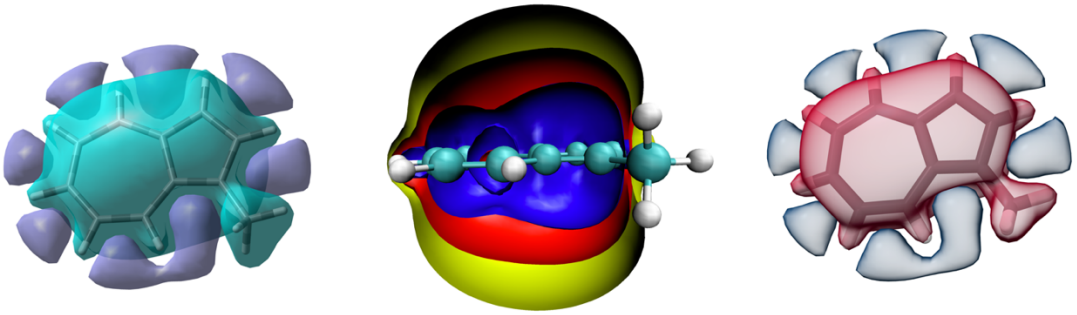
```
Please wait...
ICSScub3D is extracting magnetic shielding tensor from the output files...

Processing /Users/tetsu/Desktop/example/methylazulene_3DICSS_0001.log...
Processing /Users/tetsu/Desktop/example/methylazulene_3DICSS_0002.log...
…
Processing finished!
```

4) Choose the component of ICSS plot. User can choose from isotropic, anisotropic, and 9 XYZ components of magnetic shielding tensors from the menu.

```
Choose shielding tensor for 3D-ICSS map:
     1 - Isoptropic      2 - Anisotropy
     3 - XX component    4 - YX component    5 - ZX component
     6 - XY component    7 - YY component    8 - ZY component
     9 - XZ component   10 - YZ component   11 - ZZ component
```

```
      Please input the No.: 11
```

5) The *.cub* file including ICSS tensors would be generated in the same dictionary as the output files. You can visualize it with *GaussView*, *VMD*, *ChimeraX*, etc.



GaussView
iso = 6.56

VMD
iso = –20, –10, –5

ChimeraX
iso = 6.56