ICSScsv

powerd by python

ICSScsv Manual

Extract magnetic shielding tensor from ICSS output, version 1.0

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

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[ICSScsv Website]

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

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1. Overview

1.1 About ICSScsv

ICSScsv is a program for extracting magnetic shielding tensor from ICSS calculation output. ICSScsv is written in Python 3, thus, users can run ICSScsv through Python IDE. The executable files for macOS, Linux and Microsoft Windows operating systems are provided, users can easily run ICSScsv on any platform.

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

1.2 How it Works

ICSScsv reads an output file of ICSS calculation and extracted shielding tensor from it. ICSScsv prints the data out in *.csv* file, user can open it with data process software like *Origin*, *Prism* or even *Excel* to plot the ICSS map.

2. Install/Run ICSScsv

2.1 Run with Source Code

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

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

```
python3 /path_to_ICSScsv/ICSScsv_v10_source.py
```

2.2 Run on macOS with Executable File

All executable files are packaged in *execufiles.zip*.

2.2.1 Use Packaged Executable File

The pre-packaged executable file "*ICSScsv_v10_mac*" should be running normally on macOS 10.15 or newer with Intel and Apple M1 chip. You can run ICSScsv by double click and ICSScsv 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 ICSScsv by yourself.

1) Open terminal, execute `pip3 install pyinstaller` to install necessary packages.
2) Assume the source code file is located "*/home/user/ICSScsv/ICSScsv_v10_source.py*", execute command below.

```
pyinstaller /home/user/ICSScsv/ICSScsv_v10_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 ICSScsv by double clicking.

2.3 Run on Linux with Executable File

1) Assume the executable file is located "*/home/user/ICSScsv/execufiles/ICSScsv_v10_linux*", run below command to add executable permission to it.

```
chmod +x /home/user/ICSScsv/execufiles/ICSScsv_v10_linux
```

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

```
alias ICSScsv=/home/user/ICSScsv/execufiles/ICSScsv_v10_linux
```

3) After re-entering the terminal, and you can run ICSScsv at any dictionary by execute "`ICSScsv`" command. If you passed the step (2), you need to execute the full path to *ICSScsv_v10_linux* for running it.

2.4 Running on Microsoft Windows with Executable File

Find "*ICSScsv_v10_win.exe*" file in program folder, double click it and ICSScsv will be running in command line window.

3. How to Use

3.1 Before Running

You need prepare a Gaussian output file (*.log* or *.out*) of ICSS calculation. You can use ICSSgen (http://www.wangzhe95.net/program-icssgen) to create an input file for ICSS calculation. An example out file of benzene is attached in *example* folder, the input file of this example can be found in homepage of ICSSgen:

3.2 Process ICSS Output

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

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

```
Please specify the Gaussian output file path:
(eg.: /ICSScsv/example/benzene.log)
/Users/path_to_ICSScsv/example/benzene_ICSS_XY_0.log
```

2) Choose which component will be used for ICSS map. Please input the number of the component, and press enter.

```
Choose shielding tensor for 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
```

3) A *.csv* file including shielding tensor data would be generated in the same dictionary as the Gaussian output file, named with "*xxx_output_component.csv*". ICSScsv termination.

3.3 After Running

Open the ICSScsv output *.csv* file with data process software like Origin, Prism, etc.