ICSScsv

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ICSScsv Manual

Extract magnetic shielding tensor from ICSS output, version 3.1

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

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[*ICSScsv* Website]

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

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.

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 and plots the 2D-ICSS map with *matplotlib*, user can open it with data process software like *Origin*, *Prism* or even *Excel* to plot the ICSS map. If you don't have such data process software, *ICSScsv* also saves the *.png* file plotted with *matplotlib* at same folder.

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). CSIgen is running with external library *openpyxl*, please make sure *openpyxl* is already installed on your PC before running CSIgen. (Users can execute `pip3 install openpyxl` in terminal/command line window to install it.)

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

3.1 Before Running

You need prepare a *Gaussian* (Gaussian Inc.) 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.

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:

            (e.g.: /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*", along with a *.png* image in same name.

3.3 After Running

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