CSIgen Manual

Computational Supporting Information generator

---------- 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-csigen

1. Overview

CSIgen is a Python program for generating computational supporting information (CSI) easily. CSIgen are open-source, free, high-efficient, and user-friendly. We provide the executable files for macOS/Linux and Microsoft Windows, and the source code.

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

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

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

3.1 Usage of CSIgen

1) Run CSIgen and drag the *Gaussian* output file to the command line window. CSIgen support output files for optimization (`opt`), frequency (`freq`, `opt+freq`) and single point (`sp`) calculations. Other output files (like `NMR`, `Scan`, `IRC`, etc) maybe able to be read by CSIgen but use with caution.

```
Please specify the Gaussian output file path:
(e.g.: /CSIgen/example/DR3b_CS2021.log)
/Users/wangzhe/Desktop/DR3b_CS2021.log
```

2) Choose the SI style by inputting the menu number. About different in each style, please refer to section **3.2**.

```
                SI Style
-----------------------------------
   1 - Full (.txt)
   2 - Simple (.txt)
   3 - Coordinates only (.txt)
   4 - Full (.xlsx)
   5 - Simple (.xlsx)
   6 - Coordinates only (.xlsx)
-----------------------------------
Please input style number: 4
```

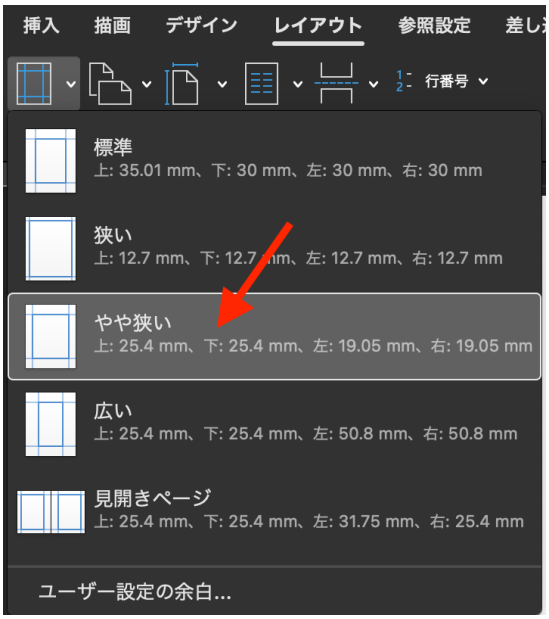
3) SI file will be saved as *.txt* (style 1~3) or *.xlsx* (style 4~6) at same dictionary as the *Gaussian* output file.

3.2 Template in CSIgen

CSIgen provides 6 built-in templates: full information, simplified information and coordinates only for text file (*.txt*) and *Excel* table file (*.xlsx*).

Full information templates include routine line, charge, spin multiplicity, point group, electronic energy. For frequency calculation jobs, number of imaginary frequencies, lowest imaginary frequency (if yes), and thermodynamic parameters (zero-point energy, thermal energy, enthalpies and thermal free energy) are also included. Geometry coordinates in Cartesian will be saved in the end of file. For Excel style (No. 4), a place is left blank for inserting the geometry image.

The SI style template No.4 is designed for copying and pasting into *Word* file. If you modify the margins of *Word* file to **moderate**, the SI (style No.4) can just fit to the size of the *Word* file. (See following figure and table: the table was pasted from *Excel* without further modification, the margins of this manual file is **moderate**.)



methane

Insert molecular geometry here.	`#p opt freq rb3lyp/6-31g(d)` Charge = 0, Multiplicity = 1, Point group = TD Electronic Energy = -40.518383 Hartree Number of imaginary frequencies = 0 Sum of electronic and zero-point Energies = -40.473181 Hartree Sum of electronic and thermal Energies = -40.470317 Hartree Sum of electronic and thermal Enthalpies = -40.469373 Hartree Sum of electronic and thermal Free Energies = -40.490505 Hartree

	Cartesian Coordinates				Cartesian Coordinates		
Atoms	***X***	***Y***	***Z***	**Atoms**	***X***	***Y***	***Z***
C	0.000000	0.000000	0.000000	H	0.631339	0.631339	0.631339
H	-0.631339	-0.631339	0.631339	H	-0.631339	0.631339	-0.631339
H	0.631339	-0.631339	-0.631339				

The information of imaginary frequencies and thermodynamic parameters are removed in the simplified templates.

In the coordinates only templates, no other information except geometric Cartesian coordinates.