ICSSgen and ICSScsv: Python programs for 2D-ICSS calculations

Zhe Wang[*1] **and Runzhao Guo**[2]

1 Department of Chemistry, Graduate School of Science, Hiroshima University, Hiroshima 739-8526, Japan **2** Program of Biomedical Science, Graduate School of Integrated Sciences for Life, Hiroshima University, Hiroshima 739-8526, Japan

Statement of need

2D isochemical shielding surface (2D-ICSS) maps, also known as 2D-NICS (nuclear independent chemical shift) maps, are useful tools for investigating the aromaticity of cyclic molecules (Klod & Kleinpeter, 2001; Liu et al., 2019; Miyazawa et al., 2021). A large number of ghost atoms, in addition to the target molecules, must be included in the input file for 2D-ICSS calculations. After completing the calculations, the magnetic shielding tensors of all ghost atoms must be extracted from the output files. This process is a huge and tiresome task; therefore, we present `ICSSgen` and `ICSScsv`, two open-source, highly efficient, and user-friendly Python programs, to easily generate 2D-ICSS maps.

Summary

`ICSSgen`

`ICSSgen` is a program that generates input files for high-quality 2D-ICSS calculations. Users must provide an original input file that includes the target molecular geometry and calculation method. `ICSSgen` reads the necessary information from the original input file and user-specified parameters from the command line window (e.g., plane, range, and grid quality) and adds ghost atoms to the new 2D-ICSS input file.

`ICSScsv`

`ICSScsv` automatically reads the molecular geometry and necessary parameters from the output file for the 2D-ICSS maps. Most importantly, it can extract the shielding tensor of ghost atoms and save them as a *.csv* data file. The 2D-ICSS map can be easily plotted with *.csv* files using data processing software (e.g., Origin, Prism, etc.).

Demonstrations

To illustrate the functions of `ICSSgen` and `ICSScsv`, an example of calculating the 2D-ICSS map of benzene is presented in this section.

Before running ICSSgen, the original input file is prepared:

*Corresponding author

```
#p nmr=giao rb3lyp/6-31g(d)

Benzene_optimized

0 1
...Cartesian coordinates...
```

Run ICSSgen and specify the calculation parameters (user-inputted commands are marked in italics):

```
Please specify the plane for ICSS map (XY, XZ, YZ): XY
Please input the altitude over the plane (in angstrom): 1
Please specify the range of X axis (in angstrom, e.g., -10 10): -3.5 3.5
Please specify the range of Y axis (in angstrom, e.g., -8 8): -3.5 3.5
Please specify the grid quality (value smaller than 0.25 is recommended):
(press Enter to use default value 0.2) (Enter)
ICSSgen will use grid quality of 0.2.
```

A new input file for the 2D-ICSS calculation was generated in the current dictionary. In this example, ghost atoms were added at the XY plane at an altitude of Z=1, in the range of X[-3.5, 3.5] Y[-3.5, 3.5] in a grid size of 0.2 (Figure 1).

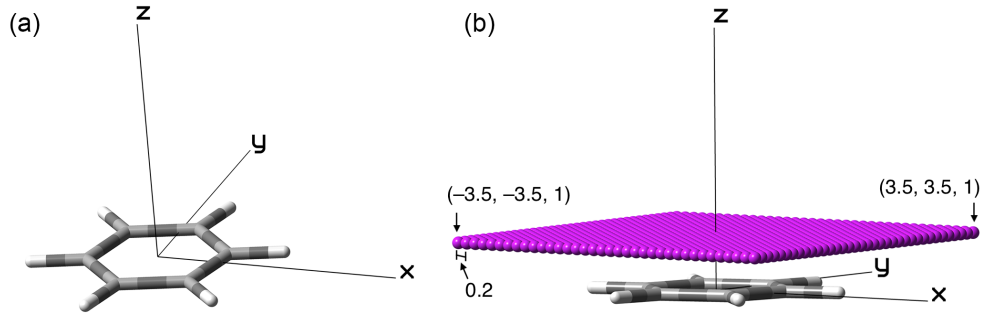

Figure 1: Geometries of (a) benezene from original input file and (b) benezene for 2D-ICSS calculation generated with ICSSgen.

After completing the 2D-ICSS calculation using Gaussian 16 (Revision B.01, M. J. Frisch, et al., Gaussian, Inc., Wallingford CT, 2016.), the output file (*.out* or *.log*) was loaded into ICSScsv, and the component used for the 2D-ICSS map was selected:

```
Gaussian output read!
ICSS will be mapped on XY plane in X[-3.5 3.5, 0.2], Y[-3.5 3.5, 0.2].

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.:
```

`ICSScsv` extracts shielding tensors of ghost atoms from the output file and summarizes them to a *.csv* data file. In Figure 2, the 2D-ICSS map was visualized using the ZZ component of the shielding tensor with OriginPro 2021 (Figure 2). Aromaticity of benzene has been will produced by 2D-ICSS map.

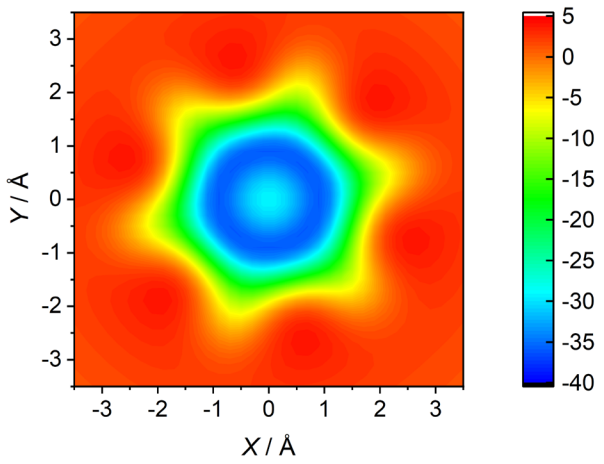

Figure 2: 2D-ICSS map of benzene visualized by OriginPro 2021.

Dependencies

`ICSSgen` and `ICSScsv` only support the Gaussian (Gaussian, Inc.) input and output.

Author informations

Zhe Wang (0000-0002-9996-586X) - Corresponding author, E-mail: wongzit@yahoo.co.jp

Runzhao Guo (0000-0002-0403-4625) - E-mail: grzsherry3090@gmail.com

References

Klod, S., & Kleinpeter, E. (2001). Ab initio calculation of the anisotropy effect of multiple bonds and the ring current effect of arenes–application in conformational and configurational analysis. *J. Chem. Soc., Perkin Trans. 2*, 1893–1898. https://doi.org/10.1039/b009809o

Liu, C., Ni, Y., Lu, X., Li, G., & Wu, J. (2019). Global Aromaticity in Macrocyclic Polyradicaloids: Hückel's Rule or Baird's Rule? *Acc. Chem. Res.*, *52*, 2309–2321. https://doi.org/10.1021/acs.accounts.9b00257

Miyazawa, Y., Wang, Z., Matsumoto, M., Hatano, S., Antol, I., Kayahara, E., Yamago, S., & Abe, M. (2021). 1,3-Diradicals Embedded in Curved Paraphenylene Units: Singlet versus Triplet State and In-Plane Aromaticity. *J. Am. Chem. Soc.* https://doi.org/10.1021/jacs.1c01329