NICSgen

powerd by python

NICSgen Manual

Input file generator for NICS calculation, version 1.1

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

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1. Overview

1.1 About NICSgen

NICSgen is an input file generator for NICS calculation. NICSgen is open-source, free, high-efficient, and user-friendly. NICSgen supports macOS, Linux and Microsoft Windows operating systems. Source code of NICSgen is also provided, thus, users can run NICSgen through Python IDE.

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

1.2 How it Works

NICSgen reads an input file including the target molecular coordinates and adds ghost atom Bq to the end of the input file. User can define the plane and altitude from NICSgen.

2. Install/Run NICSgen

2.1 Run with Source Code

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

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

```
python3 /path_to_NICSgen/NICSgen_v11_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 "*NICSgen_v11_mac*" should be running normally on macOS 10.15 or newer with Intel and Apple M1 chip. You can run NICSgen by double click and NICSgen 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 NICSgen by yourself.

1) Open terminal, execute `pip3 install pyinstaller` to install necessary packages.
2) Assume the source code file is located "*/home/user/NICSgen/NICSgen_v11_source.py*", execute command below.

```
pyinstaller /home/user/NICSgen/NICSgen_v11_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 NICSgen by double clicking.

2.3 Run on Linux with Executable File

1) Assume the executable file is located "*/home/user/NICSgen/execufiles/NICSgen_v11_linux*", run below command to add executable permission to it.

```
chmod +x /home/user/NICSgen/execufiles/NICSgen_v11_linux
```

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

```
alias NICSgen=/home/user/NICSgen/execufiles/NICSgen_v11_linux
```

3) After re-entering the terminal, and you can run NICSgen at any dictionary by execute "`NICSgen`" command. If you passed the step (2), you need to execute the full path to *NICSgen_v11_linux* for running it.

2.4 Running on Microsoft Windows with Executable File

Find "*NICSgen_v11_win.exe*" file in program folder, double click it and NICSgen will be running in command line window.

3. How to Use

3.1 Before Running

You need prepare a Gaussian input file (*.gjf* or *.com*) including route section, and molecular coordinates. Please notice that **only Cartesian coordinates is allowed**. An example input file of biphenyl is attached in *example* folder:

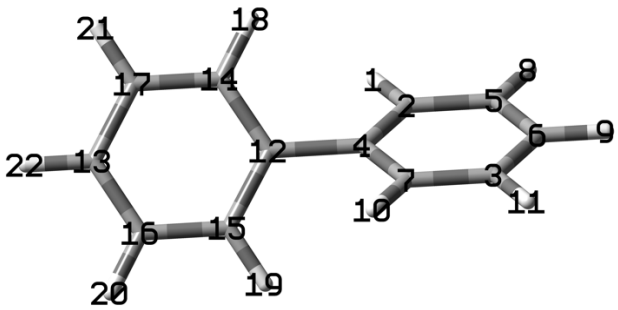
3.2 Generate NICS Input

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

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

```
Please specify the original input file path:
(eg.: /NICSgen/example/biphenyl.gjf)
/Users/path_to_NICSgen/example/biphenyl.gjf
```

2) Specify the plane which ring would be investigated. Please input 3 or more atoms number (as defined in input file). For example, ghost atoms would be added in the phenyl ring, C12-C14-C17-C13-C16-C15, thus, you can input 13 14 15 or 12 16 17 or 12 13 14 15 16 17 (non-order sensitive). Please be notice that, the Bq(0) atom would be added in the center of user-inputted atoms, for example, if 13 15 16 is inputted, the Bq(0) would be located at the center of triangle C13-C15-C16.




```
Please specify the target atoms number:
13 14 15
```

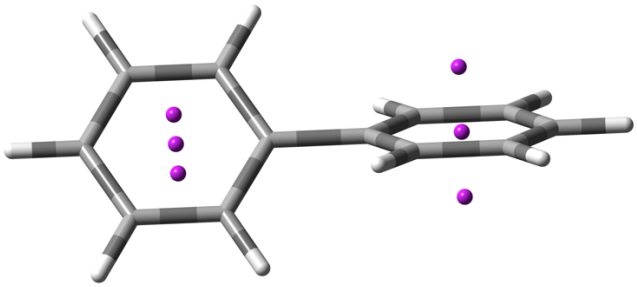
3) Specify the altitude over the ring plane. The altitude is defined in Å.

```
Please specify the altitude n of NICS(n):
1
```

4) If you want to add Bq atoms for other rings, like C2-C4-C7-C3-C6-C5, please input "*y*" and press enter, or input "*n*" to quit the program.

```
Continue to add other Bq atoms? (y/n):
y
```

5) A new input file for NICS calculation would be generated in the same dictionary as original input file, named with "*xxx_NICS.gjf*". NICSgen termination.



3.3 After Running

Open the NICS input file with text editor, and check input syntax. Then, submit it to Gaussian calculation.