HOMAcalc

powerd by python

HOMAcalc Manual

A HOMA calculator, version 1.0

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

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[*HOMAcalc* Website]

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

1. Overview

1.1 About *HOMAcalc*

HOMAcalc is a HOMA (Harmonic oscillator model of aromaticity) calculator. *HOMAcalc* is open-source, free, high-efficient, and user-friendly. *HOMAcalc* supports macOS, Linux and Microsoft Windows operating systems. Source code of *HOMAcalc* is provided, thus, users can run *HOMAcalc* through Python IDE.

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

1.2 How it Works

HOMAcalc reads optimized structure from *Gaussian* (*Gaussian* Inc.) output file (opt/freq/opt+freq) and calculate bond length from Cartesian coordinates. User can specify the atom numbers of a cyclic structure to calculate its HOMA value.

HOMAcalc use bellow equation to calculate the HOMA value with default values (*Chem. Rev.*, **2014**, *114*, 6383) of $a = 98.89$ and $R_{opt} = 1.397$ Å. User can change the value of a and R_{opt} in the program.

$$\mathrm{HOMA} = 1 - \frac{\alpha}{n}\sum_{i}^{n}\left(R_{\mathrm{opt}} - R_i\right)^2$$

1.3 Testing Platform

HOMAcalc has been tested on following platform.

1.3.1 macOS

(1) Mac mini (2020)

CPU: Intel Core i5-8500B 3.00 GHz 6 Cores 6 Threads

Mem: 16 GB 2666 MHz DDR4

GPU: Intel UHD Graphics 630 1536MB

OS: macOS 11.3.1(20E241)

(2) MacBook Air (M1, 2020)

CPU: Apple Silicon M1 8 Cores

Mem: 8 GB

GPU: Apple Silicon M1 8 Cores

OS: macOS 11.4(20F71)

1.3.2 Microsoft Windows

(1) Home-built PC I

CPU: Intel Core i7-9700KF 3.60 GHz 8 Cores 8 Threads

Mem: 16 GB 2666 MHz DDR4

GPU: Nvidia RTX 3060 12GB

OS: Windows 10 Education 20H2

(2) Home-built PC II (Physical machine with Windows/Linux dual-boot)

CPU: Intel Core i7-10700 2.90 GHz 8 Cores 16 Threads

Mem: 32 GB 2666 MHz DDR4

GPU: Intel UHD Graphics 630 1536MB

OS: Windows 10 Education 20H2

(3) Mac mini (2020) (Running with Parallels Desktop 16)

CPU: Intel Core i5-8500B 3.00 GHz 6 Cores 6 Threads (2 Cores used)

Mem: 16 GB 2666 MHz DDR4 (4 GB used)

GPU: Intel UHD Graphics 630 1536MB

OS: Windows 10 Education 1909

1.3.3 Linux

(1) Home-built PC I (Running with VMware Workstation Player 16)

CPU: Intel Core i7-9700KF 3.60 GHz 8 Cores 8 Threads (6 Cores used)

Mem: 16 GB 2666 MHz DDR4 (12 GB used)

GPU: Nvidia RTX 3060 12GB

OS: CentOS 8.3

(2) Home-built PC II (Physical machine with Windows/Linux dual-boot)

CPU: Intel Core i7-10700 2.90 GHz 8 Cores 16 Threads

Mem: 32 GB 2666 MHz DDR4

GPU: Intel UHD Graphics 630 1536MB

OS: Red Hat Enterprise Linux 8.3

(3) Mac mini (2020) (Running with Parallels Desktop 16)

CPU: Intel Core i5-8500B 3.00 GHz 6 Cores 6 Threads (3 Cores used)

Mem: 16 GB 2666 MHz DDR4 (4 GB used)

GPU: Intel UHD Graphics 630 1536MB

OS: Ubuntu 20.04, Fedora 34 beta

2. Run *HOMAcalc*

2.1 Run with Source Code

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

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

```
python3 /path_to_HOMAcalc/HOMAcalc_v*.py
```

2.2 Run with Executable File

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

2.2.1 Use Packaged Executable File

The pre-packaged executable file "*HOMAcalc_ v*_ mac*" should be running normally on macOS 10.15 or newer with Intel and Apple M1 chip. You can run *HOMAcalc* by double click the icon and *HOMAcalc* 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 *HOMAcalc* by yourself:

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

```
pyinstaller /home/user/HOMAcalc/HOMAcalc_v*_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 *HOMAcalc* by double clicking.

2.3 Run on Linux with Executable File

1) Assume the executable file is located at "*/home/user/HOMAcalc/execufiles/HOMAcalc_ v*_ linux*", run below command to add executable permission to it.

```
chmod +x /home/user/HOMAcalc/execufiles/HOMAcalc_v*_linux
```

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

```
alias homacalc=/home/user/HOMAcalc/execufiles/HOMAcalc_v*_linux
```

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

2.4 Running on Microsoft Windows with Executable File

Find "*HOMAcalc_ v*_ win.exe*" file in program folder, double click it and *HOMAcalc* will be running in command line window.

If the Windows Defender stop the *HOMAcalc*, please add the *HOMAcalc* to the safe file list. More details please check:

https://faq.nec-lavie.jp/qasearch/1007/app/servlet/relatedqa?QID=018507

3. How to Use

1) Run *HOMAcalc*, the *HOMAcalc* will request the path for *Gaussian* output file. You can drag the file into the command window or input the full path to the output file. User-inputted command are colored in red.

```
Please specify the Gaussian output file path:
(e.g.: /HOMAcalc/example/4cpp.log)
/Users/wangzhe/Desktop/4cpp.log
```

2) If you want to change the parameters (a and R_{opt}), please input `para`, and following the instruction in command window to modify the parameters. If not, go to step 3).

```
Please input the atom numbers, separated by space:
(for changing parameters, please input 'para'.)
(e.g.: 1 2 3 4 5 6)
para
-------------------------------------
     Aplha (default: 98.89)
     R_opt (default: 1.397
-------------------------------------
Specify the alpha value:
98.00
Alpha = 98.0
Specify the Ropt value:
1.399
Ropt = 1.399
```

3) Specify the atom number of cyclic structures. An example of [4]CPP is presented in following, the atom number (label) is marked on carbon atoms, hydrogen atoms are omitted.

Input the atom numbers in the bond-connecting order of cyclic structure, the numbers should be separated by

space. For example, for the ring C1-C4-C5-C2-C6-C3, please input "1 4 5 2 6 3", or "4 5 2 6 3 1", or "6 2 5 4 1 3" ..., rather than "1 2 3 4 5 6". By press ENTER key, the HOMA value would be displayed on the command window. You can calculate HOMA for other cyclic ring by input the atom number, or input "q" to terminate the *HOMAcalc*.

```
Please input the atom numbers, separated by space:
(for changing parameters, please input 'para'.)
(e.g.: 1 2 3 4 5 6)
1 4 5 2 6 3

HOMA value of ring [1 4 5 2 6 3] is 0.9842.

Input atom numbers to calculate for other ring,
or input 'q' to quit HOMAcalc.
35 32 36 33 31 34

HOMA value of ring [35 32 36 33 31 34] is 0.9842.

Input atom numbers to calculate for other ring,
or input 'q' to quit HOMAcalc.
q
```