

Introduction

The tool name is **HMG.A1**, which is free-ware software developed in Python. **HMG.A1** can run on the Microsoft Windows system. The small tool runs on nearly all operating systems with minimum requirements. The file size is less than 8 MB. It is composed of a main module where you can obtain all of the necessary operations at the end through a single-page user interface.

Training Manual

You can obtain your Homo and Lumo values after performing the necessary calculations in quantum chemistry software like Gussian, Gamess, and Pis4. The list is available on the website too. After obtaining the desired value, you can manually enter two integer values.

Within a couple of seconds, the following six results are prompt ionisation energy, electron affinity, hardness, chemical potential, electronegativity, softness, and electrophilicity index.

HMG.A1 generates output in the form of a text file. Which can easily be done with any text reader software and display results on a computer screen, which is acceptable for monochromatic vision issues, system-generated time is displayed in a text file.

Instruction Manual

You can download HMG.A1 from the GitHub website. There is a single exe file with the name of the software. Double-click the opaque icon to run this file. The tool is a virus- and bug-free programme; kindly see the **MIT** license too. If the operating system is identified as a bug, disable your computer's antivirus software for a movement and enable it after installation.

Enter a numeric value without entering the alphabet or SI unit; do not enter a blank or 0 value. Entering the same value will show a zero result, and the tool will close automatically. The system automatically generates a text file with a name result near the Exe file.

Graphical representation of HMG.A1

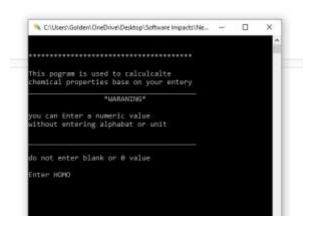


Step 1



Click on the HMG.A1.exe file.

Step 2



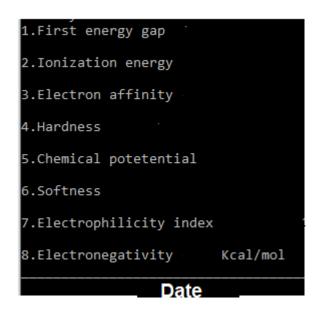
A black back ground screen will open and ask you to enter Homo value

Step 3



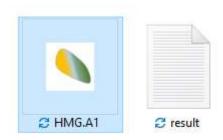
After this you will enter a Lumo value.

Step 4



Within couple of seconds following result are generated

Step 5



You can copy your finding in text file name result

Download manual

I'd be happy to help you with downloading instructions, download .exe file from github through window operating system. Launch your preferred web browser (e.g., Google Chrome, Mozilla Firefox, Microsoft Edge) etc.

Step i

You can easily download HMG.A1.exe file from the Github website by double clicking to below mention link. Web browser navigate to desire page. Locate the repository that contains the .exe file you want to download after this hit mouse button to .exe file

Link XXXXXXX



Click on a view raw

Step ii

Your browser will prompt you to choose a location on your computer to save the .exe file. Select a location and click "Save" .Another pop up ask you where to save , save a file . Depending on your's internet connection, it may take few min for the download to complete. You can monitor the progress in your browser.



Step iii

Although HMG.A1 is virus and bug free, it's a good practice to scan it for viruses using your antivirus software.

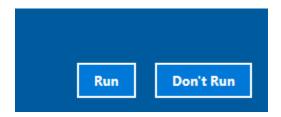
Step IV

Download is complete and you've scanned it for viruses, you can run the downloaded .exe file to install or use the application. , click on more info



Step v

That's it! You've successfully downloaded an HMG.A1.exe file from GitHub on a Windows operating system then click on run. After this follow step 1 of instruction manual.



Term of use

This software provided to under MIT licenses .Cite the software HMG.A1 if you used in your research, to generate molecular data.

Code metadata

Current code version .A1

Permanent link to code/repository used for this code version https://github.com

Permanent link to Reproducible Capsule

Legal Code License MIT

Code versioning system used git

Software code languages, tools, and services used Python 3.12

Compilation requirements, operating environments & dependencies Python

If available Link to developer documentation/manual

Yes in text and video

Support email for questions regarding to code issue <u>aziz1sh@hotmail.com</u>