

Monstergauss

Author

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Homepage

The author's homepage contains sources, documentation, additional conversion programs and lots of other usefull stuff.

<http://crc.rubberchickencult.ca/~mikep/MG/>

Source

Source code is available in the project homepage.

<http://crc.rubberchickencult.ca/~mikep/MG/>

Reference

Peterson, M., Poirier, R.: MonsterGauss. Department of Chemistry, University of Toronto, Canada (1980).

Description & Use

Monstergauss performs ab initio calculations.

Quick start

Structure of a typical input file includes e.g.:

```
*MOL BA=[basis] [other options]
(blank line)
[charge] [multiplicity]
[Z-matrix in Gaussian style]
(blank line)
...
```

Use in command line / shell:

```
gausstst < [input file] > [output file]
(in Windows command line)
```

or

```
./gausstst < [input file] > [output file]
```

(in Android shell).

The result will appear in the same location.

Note: The program is currently not able to run CI calculations (bug in the code - under study).

Program status

The current package contains MONSTERGAUSS binaries of primary version compiled for x86 based Windows operating system.

License

Monstergauss

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MinGW

The Windows version contains few essential dynamic link libraries which are part of MinGW runtime.
<http://www.mingw.org/>

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X11-Basic

GUI of the Windows version was built using X11-Basic (by Markus Hoffmann) framework (GPL v.3). For correct functionality, SDL library (available under GNU LGPL license) is included in package.

<http://x11-basic.sourceforge.net/>

<https://www.libsdl.org/>

Advanced Installer

The MSI installer for Windows was created using the Advanced Installer (Freeware edition).

<https://www.advancedinstaller.com/>

<https://www.advancedinstaller.com/top-freeware-features.html>

Contact

Compilation of the source code for Android/Windows as well as the Android/Windows app development was done by Alan Liška (alan.liska@jh-inst.cas.cz) and Veronika Růžicková (sucha.ver@gmail.com), J. Heyrovský Institute of Physical Chemistry of the CAS, v.v.i., Dolejškova 3/2155, 182 23 Praha 8, Czech Republic.

Website: <http://www.jh-inst.cas.cz/~liska/MobileChemistry.htm>