MOPAC

Author

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Homepage

The official website of MOPAC® is maintained by Stewart Computational Chemistry.
http://openmopac.net/

Source

The official sources (up to MOPAC 7.1) are available in the official website.
http://openmopac.net/
More recent versions (MOPAC2007, MOPAC2009, MOPAC2012, MOPAC2016) are not open-source.
There is plenty of other sites which distribute some flavour of MOPAC - CCL archives, funet archives, SourceForge, GitHub etc.
http://www.ccl.net/cca/software/MS-DOS/mopac_for_dos/index.shtml
http://www.nic.funet.fi/pub/sci/chem/qcpe/mopac6.0/
https://sourceforge.net/projects/mopac7/
https://github.com/metapfhor/MOPAC

Reference

Stewart, James J.P., Journal of computer-aided molecular design 4(1) (1990) 1-103.

Description & Use

MOPAC is one of the most favourite and well-known semiempirical package which enables MNDO, MINDO/3, AM1 and PM3 calculations.

Quick start

A typical input file contains:

```
Keywords
Description
(blank line)
[atom] [x] [1 or 0] [y] [1 or 0] [z] [1 or 0]
...
(blank line)
(blank line)
```

The input file is saved as FOR005 to the folder where the MOPAC executable is present.

Use in command line / shell:

`mopac` (in Windows command line)

or

`./mopac` (in Android shell).

The result named FOR006 will appear in the same location. It should be noted that any files other than FOR005 must be removed from the folder before executing a new calculation.

Program status

The current package contains MOPAC 7 binaries of primary version compiled for the particular Android hardware platforms and adapted for running in terminal environment.

License

MOPAC7

The distribution is published as freeware at Mobile Chemistry Portal and Google Play Store with kind permission of James Stewart. We are also grateful to metapfhor (GitHub, https://github.com/metapfhor/MOPAC) for ready-to-compilation form of MOPAC 7 source code.

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```

MinGW

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

```
Copyright (c) 2012 MinGW.org project

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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

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