MOPAC with COSMO support

Authors

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Homepage

The official website of MOPAC® is maintained by Stewart Computational Chemistry.
http://openmopac.net/
The COSMO modification of the original code is described here.
https://github.com/brhr-iwao/MOPAC7SP

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
The patched source used for this distribution was taken from:
https://github.com/brhr-iwao/MOPAC7SP

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 [input file].dat (or with other name) to the folder where the MOPAC executable is present.

Use in command line / shell:

`mopac` [input file]`.dat` (in Windows command line)

or

`./ mopac` [input file]`.dat` (in Android shell).

The output file(s) will appear in the same location.

Program status

The current package contains MOPAC-COSMO binaries based on MOPAC 7 compiled for x86 based Windows operating system.

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 Aoyama Iwao (GitHub, https://github.com/brhriwao/) for ready-to-compilation form of patched 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/

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 Růžičková (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