MOPAC with PDDG support

Authors

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Homepage

The official website of MOPAC® is maintained by Stewart Computational Chemistry.
http://openmopac.net/
The PDDG modification of the original code is described here.
http://zarbi.chem.yale.edu/doc/pddg/

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.
Repasky, Matthew P., Chandrasekhar, J., Jorgensen, W.L., Journal of computational chemistry 23(16)
(2002) 1601-1622.

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-PDDG binaries based on MOPAC 6 compiled for x86 based Windows operating system.

License

MOPAC6

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

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

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