

# MOPAC with PDDG support

## Authors

James J.P. Stewart (MOPAC 7)  
Matt Repasky (PDDG extension)

## 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.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 the particular Android hardware platforms and adapted for running in terminal environment.

## License

### MOPAC6

The distribution is published as freeware at Mobile Chemistry Portal and Google Play Store with kind permission of James Stewart and Julian Tirado-Rives. We are also grateful to metaphor (GitHub, <https://github.com/metaphor/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/>

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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>