

# MOPAC with PDDG support

## Authors

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

## Homepage

The official website of MOPAC<sup>®</sup> 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.

```
THE SOFTWARE IS PROVIDED "AS IS", WITHOUT WARRANTY OF ANY KIND, EXPRESS
OR IMPLIED, INCLUDING BUT NOT LIMITED TO THE WARRANTIES OF
MERCHANTABILITY, FITNESS FOR A PARTICULAR PURPOSE AND NONINFRINGEMENT.
IN NO EVENT SHALL THE AUTHORS OR COPYRIGHT HOLDERS BE LIABLE FOR ANY
CLAIM, DAMAGES OR OTHER LIABILITY, WHETHER IN AN ACTION OF CONTRACT,
TORT OR OTHERWISE, ARISING FROM, OUT OF OR IN CONNECTION WITH THE
SOFTWARE OR THE USE OR OTHER DEALINGS IN THE SOFTWARE.
```

## 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

Permission is hereby granted, free of charge, to any person obtaining a copy of this software and associated documentation files (the Software"), to deal in the Software without restriction, including without limitation the rights to use, copy, modify, merge, publish, distribute, sublicense, and/or sell copies of the Software, and to permit persons to whom the Software is furnished to do so, subject to the following conditions:

The above copyright notice, this permission notice and the below disclaimer shall be included in all copies or substantial portions of the Software.

THE SOFTWARE IS PROVIDED "AS IS", WITHOUT WARRANTY OF ANY KIND, EXPRESS OR IMPLIED, INCLUDING BUT NOT LIMITED TO THE WARRANTIES OF MERCHANTABILITY, FITNESS FOR A PARTICULAR PURPOSE AND NONINFRINGEMENT. IN NO EVENT SHALL THE AUTHORS OR COPYRIGHT HOLDERS BE LIABLE FOR ANY CLAIM, DAMAGES OR OTHER LIABILITY, WHETHER IN AN ACTION OF CONTRACT, TORT OR OTHERWISE, ARISING FROM, OUT OF OR IN CONNECTION WITH THE SOFTWARE OR THE USE OR OTHER DEALINGS IN THE SOFTWARE.

## 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>