

# 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.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/metaphor/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 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 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/>

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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.

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