

# OpenMolcas

## Authors

The OpenMolcas Authors (Christian Ander, Kerstin Andersson, János G. Ángyán, Francesco Aquilante, Jochen Autschbach, Jie J. Bao, Maria Barysz, Stefano Battaglia, Eugeniusz Bednarz, Nelson H. F. Beebe, Anders Bernhardsson, Margareta R. A. Blomberg, Piotr Borowski, Jonas Boström, Per Boussard, John Burkardt, Yannick Carissan, Liviu Chibotaru, Christophe Chipot, Aron Cohen, David L. Cooper, Maurizio Cossi, Joel Creutzberg, Oleh Danyliv, Mickaël G. Delcey, Ajitha Devarajan, Luca De Vico, Michael Diedenhofen, Sijia S. Dong, Thomas Dresselhaus, Daniel Fairhead, Ignacio Fdez. Galván, Nicolas Ferré, Timo Fleig, Leon Freitag, Luis Manuel Frutos, Markus P. Fülscher, Alexander Gaenko, Laura Gagliardi, Walter Gautschi, Giovanni Ghigo, Coen de Graaf, Gene H. Golub, Sergey Gusarov, Daniel Hagberg, Jun-ya Hasegawa, José Manuel Hermida-Ramón, Bernd Artur Heß, Asbjørn Holt, Chad E. Hoyer, Denis Jelovina, Marcus Johansson, Erik Källman, Gunnar Karlström, Stefan Knecht, Jesper Wisborg Krogh, Teodoro Laino, Giovanni Li Manni, Roland Lindh, Johan Lorentzon, Dongxia Ma, Yingjin Ma, Per Åke Malmqvist, Neil Martinsen-Burrell, Andy May, Manuela Merchán, Samuel Mikes, Abdul Rehaman Moughal Shahi, Thomas Müller, Takahito Nakajima, Naoki Nakatani, Pavel Neogrady, Jesper Norell, Anders Öhrn, Jeppe Olsen, Markus Oppel, Thomas Bondo Pedersen, Daoling Peng, Kurt Pfingst, Quan Phung, Michal Pitoňák, Felix Plasser, Christian Pomelli, Ben Pritchard, Juraj Raab, Markus Reiher, H. Rieger, Björn O. Roos, Ulf Ryde, Pawel Salek, Andrew M. Sand, Michael A. Saunders, Igor Schapiro, Bernd Schimmelpfennig, Martin Schütz, Luis Seijo, Luis Serrano-Andrés, Kamal Sharkas, Grigory A. Shamov, Prachi Sharma, Per E. M. Siegbahn, Pär Söderhjelm, Lasse Kragh Sørensen, Jonna Stålring, Hermann Stoll, Bingbing Suo, Ben Swerts, Akio Takatsuka, Thorstein Thorsteinsson, Takashi Tsuchiya, Liviu Ungur, Morgane Vacher, Alessio Valentini, Valérie Vallet, Steven Vancoillie, Valera Veryazov, Victor Vysotskiy, Ulf Wahlgren, Yubin Wang, Mark A. Watson, Hans-Joachim Werner, Oskar Weser, Per-Olof Widmark, Małgorzata Wierzbowska, Alexander Wolf, Sebastian Wouters, Felipe Zapata, Alexander Zech, Yan Zhao, J. Patrick Zobel), check the author page.

<https://gitlab.com/Molcas/OpenMolcas/blob/master/CONTRIBUTORS.md>

## Homepage

The project is located at GitLab.

<https://gitlab.com/Molcas/OpenMolcas>

## Source

Source code is available in the homepage.

<https://gitlab.com/Molcas/OpenMolcas>

## Reference

**Molcas 8:** J. Comput. Chem. 37 (2016) 506-541. DOI: 10.1002/jcc.24221  
**Molcas 7:** J. Comput. Chem. 31 (2010) 224-247. DOI: 10.1002/jcc.21318  
**Molcas 6:** Comput. Mat. Sci. 28 (2003) 222-239. DOI: 10.1016/S0927-0256(03)00109-5  
**Code development:** Wiley Interdiscip. Rev. Comput. Mol. Sci. 3 (2013) 143-149. DOI: 10.1002/wcms.1117; Int. J. Quantum Chem. 100 (2004) 626-635. DOI: 10.1002/qua.20166  
**Latest reference** (cited 15.12.2019): "OpenMolcas: From Source Code to Insight." J. Chem. Theory Comput. 15 (2019) 5925-5964. DOI: 10.1021/acs.jctc.9b00532

## Description & Use

OpenMolcas is a general purpose molecular electronic structure computational program which utilizes multiconfigurational approach as the key-feature.

## Quick start

Use in command line / shell:

```
pymolcas -f [name of input file]
```

(in Windows command line)

or

```
./pymolcas -f [name of input file]
```

(in Android shell).

The result will appear in the same location. (For correct functionality, a working installation of Python 3 with additional packages Setuptools, Pyparsing and Six is required. For more detailed information on configuration the environment variables, please refer to the included original manual, or type `export MOLCAS=[/path/to/your/molcas/root/directory]` followed by running `pymolcas --setup` and answering the prompts).

## Program status

The current package contains OpenMolcas binaries of a version issued within year 2019 compiled for the particular Android hardware platforms and adapted for running in terminal environment.

# License

## OpenMOLCAS

The distribution of OpenMolcas binaries as well as the compiled pymolcas execution script is published for free (under LGPL v.2.1) at Mobile Chemistry Portal and Google Play Store with kind permission of Roland Lindh. The corresponding source code for generic Android binaries is available as well.

The included documentation, basis, example and other files were taken from the official OpenMolcas source code distribution.

<https://gitlab.com/Molcas/OpenMolcas>

## TermOnePlus

The individual parts of OpenMOLCAS require for their concerted interaction and communication during computation in an Android device a fully functional terminal emulator. As the famous original Terminal Emulator by Jack Palevich is not being continuously developed up to now, we decided to use its more recent update TermOnePlus by Roumen Petrov as the versatile framework in which we placed all the OpenMolcas related stuff. TermOnePlus is released under Apache license 2.0, check the homepage for details).

<https://github.com/jackpal/Android-Terminal-Emulator>

<https://termoneplus.com/>

## Busybox

Use of OpenMOLCAS program in terminal environment of TermOnePlus benefits from availability of common Linux commands and utilities which were introduced to this project by Busybox. The Busybox binaries for Android included in the OpenMolcas installer offered by us were compiled from the source code according to Gianluigi Tiesi (alias "sherpya", check the homepage for details). Busybox is released under GPL v.2 license (check the homepage for details).

<https://github.com/sherpya/android-busybox>

<https://busybox.net/license.html>

## Cygwin

The Windows version of OpenMOLCAS binaries offered by us is embedded in Cygwin runtime environment which is licensed under GPL and LGPL licenses (check the homepage for details).

<https://cygwin.com/COPYING>

<https://cygwin.com/COPYING.LIB>

<https://cygwin.com/licensing.html>

## Python

OpenMOLCAS execution script pymolcas requires properly installed Python interpreter, therefore the OpenMOLCAS binaries offered by us for both Android and Windows are bundled with Python. Android installer of OpenMOLCAS runtime contains Python 3.7 runtime compiled using either the official Android NDK (for recent Android versions 5+) or CRYSTAX NDK for older OS versions. The Windows version contains Python 3.7 preinstalled inside of the Cygwin runtime. Python 3.7 is distributed under PSF license agreement (check the homepage for details).

<https://docs.python.org/3.7/license.html>

## Setuptools

OpenMOLCAS execution script pymolcas requires for its functionality the Python package Setuptools to be present and properly installed (released under MIT license, check the homepage for details).

<https://pypi.org/project/setuptools/>

## Pyparsing

OpenMOLCAS execution script pymolcas requires for its functionality the Python package Pyparsing to be present and properly installed (released under MIT license, check the homepage for details).

<https://pypi.org/project/pyparsing/>

## Six

OpenMOLCAS execution script pymolcas requires for its functionality the Python package Six to be present and properly installed (released under MIT license, check the homepage for details).

<https://pypi.org/project/six/1.5.0/>

## BLAS

OpenMOLCAS binaries for Android offered by us were statically linked to reference BLAS library (from the LAPACK package - released under modified BSD license, check the homepage for details). The Windows package contains the corresponding dynamic library inside of Cygwin runtime.

<http://www.netlib.org/lapack/>

## LAPACK

OpenMOLCAS binaries for Android offered by us were statically linked to LAPACK library (released under modified BSD license, check the homepage for details). The Windows package contains the corresponding dynamic library inside of Cygwin runtime.

<http://www.netlib.org/lapack/>

## Crystax NDK

OpenMOLCAS binaries for older Android versions (up to 4.4 KitKat) offered by us were compiled using the Crystax NDK, therefore they are dynamically linked to LIBCRYSTAX library (from the compiler - released under modified BSD 2 clause license, check the homepage for details).

<https://www.crystax.net/android/ndk>

## 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](mailto:alan.liska@jh-inst.cas.cz)) and Veronika Růžicková ([sucha.ver@gmail.com](mailto: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>