**ScaLAPACK**

**Description**: A subset of LAPACK routines for parallel calculations.

**Site**: http://www.netlib.org/scalapack/

**License** (Modified BSD license):

**Open MPI**

**Description**: Open Source MPI implementation (Version 3)

**Site**: https://www.open-mpi.org/community/license.php

**License** (New BSD license):

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**XCFun**

**Description**: XCFun is a library of DFT exchange-correlation (XC) functionals.

**Site**: http://dftlibs.org/xcfun/

**License**:

A modified LGPL license that allows us to link ORCA statically with XCFun.



Reference:

Ulf Ekström, Lucas Visscher, Radovan Bast, Andreas J. Thorvaldsen and Kenneth Ruud, *Arbitrary-Order Density Functional Response Theory from Automatic Differentiation*, Journal of Chemical Theory and Computation 6, 1971 (2010), DOI: 10.1021/ct100117s

**otool_smd**

**Description**: otool_smd is a standalone code that, delivered a molecular geometry, computes the CDS energies and gradients. The code is a modification of parts of the GESOL code, which is redistributed with permission of C. J. Cramer and D. G. Truhlar.

**Site**: https://comp.chem.umn.edu/gesol/

**License conditions**:

When publishing SMD results users shall cite:

Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. (2009) J. Phys. Chem. B, 113, 6378.

**References**:

GESOL Code: Marenich, A.; Hawkins, G.; Liotard, D.; Cramer, D., GESOL - version 2008. https://comp.chem.umn.edu/gesol.

SMD Publication: Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. (2009) J. Phys. Chem. B, 113, 6378.

**otool_gcp**

**Description**: otool_gcp is used as an external tool that computes an energy correction in order to remove artificial overbinding effects from BSSE.

**Site**: https://www.chemie.uni-bonn.de/pctc/mulliken-center/software/gcp/gcp

**License** :

**OpenBLAS**

**Description**: OpenBLAS is an optimized BLAS library. It is used within the Windows executables.

**Site**: https://www.openblas.net/

**License** (BSD):

**Intel® Math Kernel Library (Intel® MKL)**

**Description**: Fastest and most used math library for Intel and compatible processors.

**Site**: https://software.intel.com/en-us/intel-mkl

**License:**

https://software.intel.com/en-us/articles/end-user-license-agreement

**Libint**

**Description**: libint is a library of C/C++ functions for efficient evaluation of several kinds of two-body molecular integrals over Gaussian functions and the optimizing compiler that generates a Libint library. Libint version 2 has been integrated into ORCA.

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