

OMNISOL: A Program for Calculating Free Energies of Solvation and Air-Water Interface Adsorption Coefficients using Geometry-Dependent Atomic Surface Tensions.

Version 2.0 Manual

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ABSTRACT:

OMNISOL is a computer program for calculating free energies of solvation for molecules containing H, C, N, O, F, S, Cl, Br, and I in water and molecules containing H, C, N, O, F, P, S, Cl, Br, and I in organic solvents using the SM5.0R solvation model. In SM5.0R, all contributions to the solvation energy are based on the gas-phase geometry of the solute and a set of solvent descriptors. The solvation free energy takes the form of a sum of atomic surface tensions times solvent-accessible surface areas. The surface tensions are functions of the solute bond distances and the solvent descriptors. The solvent-accessible surface areas are functions of the solute geometry. Electrostatics and geometry relaxation are not treated explicitly but are implicit in the parameters.

In addition to calculating free energies of solvation, a utility program is included with OMNISOL that calculates adsorption coefficients at air-water interfaces using the SM5.0R-Surf model. SM5.0R-Surf works in the same way as SM5.0R (i.e. a set of geometry-dependent atomic surface tensions and a set of empirically determined solvent descriptors to describe solvent molecules at the air-water interface are used to calculate free energies), except that SM5.0R-Surf also takes into account the dimensionality change free energy associated with moving a solute from the three-dimensional vapor phase to the air-water interface, which is modeled as a homogenous, two-dimensional interface.

CONTENTS:

TITLE PAGE.....	i
CONTENTS.....	ii
USER AGREEMENT.....	iii
1. INTRODUCTION.....	1-1
2. INSTALLING OMNISOL.....	2-1
2.1 Description of the Code.....	2-1
2.2 Files in Distribution.....	2-2
2.3 Running OMNISOL on Windows.....	2-4
2.4 Execution Script.....	2-4
2.5 Installation Script.....	2-5
2.6 Installing the SM5.0R-Surf Utility Program.....	2-5
3. USAGE AND KEYWORD EXPLANATIONS.....	3-1
4. TEST RUN INPUT AND OUTPUT.....	4-1
5. OUTPUT.....	5-1
6. COMPUTERS AND COMPILERS FOR WHICH THE CODE HAS BEEN TESTED.....	6-1
6.1 Known Issues.....	6-1
6.2 Installing OMNISOL on an Apple Machine.....	6-2
7. REVISION HISTORY.....	7-1
8. ACKNOWLEDGMENTS.....	8-1

USER AGREEMENT

OMNISOL is a licensed program and use of this program implies acceptance of the terms of the license, which are repeated here for convenience:

1. No user or site will redistribute the source code or executable code to a third party in original or modified form without the written permission of one of the principal investigators (Christopher J. Cramer or Donald G. Truhlar). A license does not entitle the licensee to relicense the code or distribute it in original or modified form to parties not covered by the license. The licensee has no ownership rights in the OMNISOL software or in any copyrights of the OMNISOL software or documentation through this license. A user license covers the work of a single research group and the code may be shared and disseminated within a group without requiring permission. Site-license inquiries should be directed to either of the principal investigators.
2. Publications resulting from using this package will cite the program. The recommended reference is:

C. P. Kelly, G. D. Hawkins, B. J. Lynch, D. A. Liotard, C. J. Cramer, and D. G. Truhlar, OMNISOL-version 2.0, University of Minnesota, Minneapolis, 2005.
3. No guarantee is made that this program is bug-free or suitable for specific applications, and no liability is accepted for any limitations in the mathematical methods and algorithms used within the program.
4. No consulting or maintenance services are guaranteed or implied.

1. INTRODUCTION

OMNISOL is a computer program for calculating free energies of solvation for organic molecules containing H, C, N, O, F, S, Cl, Br, and I in water and organic solvents using the SM5.0R solvation model. In this model, all contributions to the solvation energy are based on the gas-phase geometry of the solute and a set of solvent descriptors. The solvation free energy takes the form of a sum of atomic surface tensions times solvent-accessible surface areas. The surface tensions are functions of the solute bond distances and the solvent descriptors. The solvent-accessible surface areas are functions of the solute geometry. Electrostatics and geometry relaxation are not treated explicitly but are implicit in the parameters.

The SM5.0R model used in OMNISOL is fully explained in the following three references:

1. "Parameterized Model for Aqueous Free Energies of Solvation Using Geometry-Dependent Atomic Surface Tensions with Implicit Electrostatics," G. D. Hawkins, C. J. Cramer, and D. G. Truhlar, *Journal of Physical Chemistry B* 101, 5084-5088 (1997).
2. "OMNISOL: Fast Prediction of Free Energies of Solvation and Partition Coefficients," G. D. Hawkins, D. A. Liotard, C. J. Cramer, and D. G. Truhlar, *Journal of Organic Chemistry* 63, 4305-4313 (1998).

The method used to calculate the surface areas is explained in

3. "Improved Methods for Semiempirical Solvation Models," D. A. Liotard, G. D. Hawkins, G. C. Lynch, C. J. Cramer, and D. G. Truhlar, *Journal of Computational Chemistry*, 16, 422-440 (1995).

In addition, a parameter that extends the method to phosphorus-containing compounds has been determined and is reported in

4. "Predicting Air-Water Adsorption Coefficients Using a Universal Solvation Model," C. P. Kelly, C. J. Cramer, and D. G. Truhlar, *Journal of Physical Chemistry B*, 108, 12882-12897 (2004).

Solvent properties needed for application to common solvents are provided with the code and, for the convenience of users, they are also gathered in the following database:

5. <http://comp.chem.umn.edu/solvation/mnsddb.pdf>

In addition to calculating free energies of solvation, a utility program is included with OMNISOL that calculates adsorption coefficients at air-water interfaces using the SM5.0R-Surf model. SM5.0R-Surf works in the same way as SM5.0R (i.e. a set of geometry-dependent atomic surface tensions and a set of empirically determined solvent descriptors to describe solvent molecules at the air-water interface are used to calculate free energies), except that SM5.0R-Surf also takes into account the dimensionality change free energy associated

with moving a solute from the three-dimensional vapor phase to the air-water interface, which is modeled as a homogenous, two-dimensional interface. A full description of this method is reported in ref. 4 above.

2. INSTALLING OMNISOL

2.1. Description of the Code

OMNISOL is written in very portable FORTRAN 77. (The only extension to FORTRAN 77 that is employed is the INCLUDE extension, and the only nonstandard usage is lower case file names.) The only machine-dependent routines (dateclock.c, datesv.*, porcpu.*) are included for monitoring the run time of the code and they can be easily disabled for modified for use on platforms other than those for which OMNISOL was developed. As discussed in section 6, the code also compiles correctly with FORTRAN90 compilers.

The memory requirements of the OMNISOL code can be adjusted by altering the parameter NUMATM in the SIZES.i file in the include directory. NUMATM refers to the maximum number of atoms that will be allowed in a single molecule. The default is 70 atoms. (Note: If altering the NUMATM parameter, all FORTRAN files must be recompiled before the new limits will take effect.)

2.2. Files in Distribution

This version of OMNISOL constitutes a single package that consists of the following directories and files:

Directory	File descriptions
include	This directory contains the following files that are used in conjunction with the FORTRAN INCLUDE statement:
SIZES.i	This INCLUDE file contains parameter NUMATM and related parameters that control the length of the arrays created by the OMNISOL code. NUMATM is the maximum number of atoms allowed in a run.
PARAMS.i	This INCLUDE file contains parameters that are used in the SM5.0R models.

KEYS.i This INCLUDE file includes common blocks containing all the keywords that are used in OMNISOL.

FFILES.i This INCLUDE file includes a common block which contains variables that set which FORTRAN units are used during a run.

mach This directory contains the following machine-dependent files:

dateclock.c This is a C subprogram which is used by datesv.ibm to obtain the date and time.

datesv.cray This is the date/time subprogram for Cray computers.

datesv.dec This is the date/time subprogram for DEC 3000 AXP workstations.

datesv.ibm This is the date/time subprogram for IBM RS/6000 workstations.

datesv.linux This is the date/time subprogram for Linux and Mac OSX/Darwin workstations.

datesv.iris This is the date/time subprogram for IRIS workstations.

datesv.sun This is the date/time subprogram for SUN workstations.

porcpu.cray This subprogram determines the CPU time on Cray computers.

porcpu.dec This subprogram determines the CPU time on DEC 3000 AXP workstations.

porcpu.ibm This subprogram determines the CPU time on IBM RS/6000 workstations.

porcpu.iris This subprogram determines the CPU time on IRIS workstations.

porcpu.linux This subprogram determines the CPU time on Linux and Mac OSX/Darwin workstations.

porcpu.sun This subprogram determines the CPU time on SUN workstations.

src This directory contains a series of FORTRAN77 files; each file contains one FORTRAN routine.

obj This directory is used during the compilation process to store object files.

test This directory contains a script to run OMNISOL, and it also contains the test input files. Files included are:

 omnisol.c This file is a C shell script for interactive execution of the OMNISOL program.

 omnisolv.prp This file contains preformatted keyword lines which provide the solvent properties needed to run SM5.0R-organic calculations for many common organic solvents. To use a line from the file, include the keywords for the desired solvent with the other keywords in the .dat file.

 trxx.dat This is the data file for test suite run xx. An additional 'a' after the number indicates an aqueous solvation run, and an addition 'n' indicates a non-aqueous solvation run. A total of 30 runs constitute the test suite.

testo This directory contains sample output files from OMNISOL. Files included are:

 trxx.out This is the output file for test suite run xx resulting from a run on a SGI R10000 workstation workstation.

util This directory contains the utility program for calculating air-water interface adsorption coefficients.

PC This directory contains all files required to run OMNISOL on the Windows operating system. Files include:

 omnisol1.1.exe This is the Windows executable.

 run_tests.bat This is a batch file to run all the test runs in the /test directory using the Windows executable.

 compare.pl This is a Perl script to compares all the output to the files in the /testo directory. It creates a file that describes the differences.

 omnisol.mak The make file to compile OMNISOL on Windows

 omnisol1.1.mdp The Microsoft Developer project file to easily compile OMNISOL using Fortran Powerstation

2.3 Running OMNISOL on Windows

The PC directory contains the files necessary to run OMNISOL on Windows. Double-clicking on run_tests.bat will run all the tests in the /test directory. The Perl script compare.pl will verify that the test runs give the correct results.

2.4. Execution Script

The test directory of the OMNISOL package contains a script called omnisoli.c which should be customized to work within the user's directory structure. In this script, the following statement must be changed to configure the script.

```
set omnisolexe = /fullpathnamefortheexecutablefile
```

The path name for the executable needs to be placed on the right of the equal sign. NOTE: Only relative pathnames are allowed. In other words, if the OMNISOL package is used as distributed, such that the omnisol.exe is compiled in the main directory and the omnisoli.c script is in the test directory, then the set statement should be changed as follows:

```
set omnisolexe = ../omnisol.exe
```

When using any of the run-scripts, only the root name of the data file is used. For example to start a run with the tr1.dat data file, type:

```
omnisol.c tr1
```

not

```
omnisol.c tr1.dat
```

If the .dat extension is accidentally added, the script will prompt with a message indicating that the .dat extension should not be added.

2.5. Installation Script

The C shell script `omnisol.compile` has been included to install OMNISOL on any of the Unix computers for which the code has been tested. The script assumes that the directory structure is set up as explained in Section 2.2, and it can be used to compile OMNISOL using several different methods. When `omnisol.compile` is invoked, the user is prompted to choose the appropriate machine type for compilation, and also for the executable name. The allowed machine types are: `cray`, `dec`, `ibm`, `iris`, `sgi64`, and `sun`. Next the user is given options to control the type of compilation that occurs. The user can choose either a 's'tandard optimization (all subroutines are compiled and linked into the executable), or the generation of a 'm'akefile. The standard compilation is recommended for nearly all users; the makefile is only recommended for those users familiar with makefiles who also need to recompile OMNISOL on a regular basis. Additionally, when the standard option is chosen, the user may specify whether object files are 'h'eld after compilation (default) or 'n'eatly removed. IBM users are given an additional choice - whether or not their machine uses a FORTRAN preprocessor.

2.6. Installing the OMNISOL SM5.0R-Surf Utility Program

For OMNISOL users that would also like to calculate air-water interface adsorption coefficients with the SM5.0R-Surf model, the following additional steps should be taken to install the SM5.0R-Surf Utility Program.

- 1.) Move into the directory `/util`.
- 2.) Execute the script `install.pl` by typing `./install.pl`
- 3.) This script requires the absolute path to the OMNISOL executable, as well as the name of the executable. Once this information has been supplied, the script will create another script called `kia.pl`
- 4.) To run the test job (`test.dat`), use the command `./kia.pl test.dat`
- 5.) Verify that the script is working properly by comparing the data in the resulting output file, `test.log`, to the output file `kia_test.log`, which is located under the `/testo` directory.

3. USAGE AND KEYWORD EXPLANATIONS

The first line of any OMNISOL data file (*.dat) contains the keywords to be used in the calculation. If more than one line is required for the keywords, additional lines may be used if an ampersand symbol (&) appears in the first column of any additional keyword line. The two lines following the keyword line(s) are for comments about a given run and will be echoed in the output file (*.out). The subsequent lines contain the geometry of the solute molecule in the calculation.

The OMNISOL program was designed to accept standard Cartesian coordinate input in free format with four fields per record. There is one record for each atom of the solute molecule. The first field of each record contains the atomic symbol or atomic number for the atom. The second, third, and fourth fields contain the X, Y, and Z coordinates in Angstroms for the atom. If dummy atoms are included in the Cartesian coordinates they must be designated with the symbol XX. (Note: all atomic symbol input is case insensitive.) Alternatively, the OMNISOL program will accept a standard AMSOL Z-matrix input. (For more details see the keyword AMSOLZ.)

Thirty-one examples of OMNISOL input are included in the test directory of the OMNISOL distribution package.

3.1. Keywords

Any keyword that is recognized by OMNISOL is listed alphabetically in this section.

All keywords are case insensitive.

3.1.1. Keyword ALPHA=x.xx

The ALPHA keyword specifies alpha of the desired solvent for an SM5.0R-organic calculation. ALPHA is defined to be the value that Abraham denotes a solvent molecule's ability to donate a hydrogen bond. The file omnisolv.prp in the test directory of the distributed code contains values of ALPHA for many common organic solvents. The main references for values not contained in that file are:

- [1] Abraham, M. H., Chem. Soc. Rev., (1993) 73.
- [2] Abraham, M. H.; Chadha, H. S.; Whiting, G. S.; Mitchell, R. C., J. Pharm. Sci., 83 (1994) 1085.

3.1.2. Keyword AMSOLZ

The AMSOLZ keyword specifies that the data file (.dat) will be in the standard Z-matrix format used in the AMSOL code. The OMNISOL code will directly convert the internal coordinates provided into the Cartesian coordinates utilized by OMNISOL. The optimization flags, symmetry constraints, and extraneous input elements (e.g., the charges from a specialized AMSOL data file) will be ignored.

3.1.3. Keyword BETA=x.xx

The BETA keyword specifies beta of the desired solvent for an SM5.0R-organic calculation. BETA is defined to be the value that Abraham calls the sum of beta_sub_2 and it denotes a solvent molecule's ability to accept a hydrogen bond. The file omnisolv.prp in the test directory of the distributed code contains values of BETA for many common organic solvents. The main references for values not contained in that file are:

- [1] Abraham, M. H., Chem. Soc. Rev., (1993) 73.
- [2] Abraham, M. H.; Chadha, H. S.; Whiting, G. S.; Mitchell, R. C., J. Pharm. Sci., 83 (1994) 1085.

3.1.4. Keyword DETAIL

The DETAIL keyword requests that additional details about the SM5.0R calculation be printed in the output file (*.out). This information includes the calculated solvent accessible surface area, as well as a breakdown of the components of the SM5.0R calculation. Further details of the SM5.0R method can be found in the references listed in Section 1 of this manual.

3.1.5. Keyword FACARB=x.xx

The FACARB keyword specifies the fraction of non-hydrogenic solvent atoms that are carbon atoms contained in an aromatic ring. Hence, the value must necessarily be between zero and one for all solvents. The file omnisolv.prp in the test directory of the distributed code contains value of FACARB for many common organic solvents, but it can be calculated simply for any organic solvent.

3.1.6. Keyword FEHALO=x.xx

The FEHALO keyword specifies the fraction of non-hydrogenic solvent atoms that are electronegative halogen atoms (fluorine, chlorine, and bromine). Hence, the value must necessarily be between zero and one for all solvents. The file omnisolv.prp in the test directory of the distributed code contains value of FEHALO for many common organic solvents, but it can be calculated simply for any organic solvent.

3.1.7. Keyword GAMMA=x.xx

The GAMMA keyword specifies the macroscopic surface tension of the desired solvent for an SM5.0R-organic calculation. The value of GAMMA should be in units of $\text{cal mol}^{-1} \text{Angstrom}^{-2}$. The file `omnisolv.prp` in the test directory of the distributed code contains value of GAMMA for many common organic solvents. A convenient reference for values not contained in that file is the "CRC Handbook of Chemistry and Physics", published by CRC Press. A much more complete reference is Jasper, J. J., *J. Phys. Chem. Ref. Data*, 1 (1972) 841-1009.

3.1.8. Keyword IOFR=x.xx

The IOFR keyword specifies the index of refraction of the desired solvent for an SM5.0R-organic calculation. The file `omnisolv.prp` in the test directory of the distributed code contains values of IOFR for many common organic solvents. A convenient reference for values not contained in that file is any recent edition of the "CRC Handbook of Chemistry and Physics", published by CRC Press.

3.1.9. Keyword SM5.0R

Every OMNISOL calculation requires the SM5.0R keyword which indicates that a prediction of the solvation free energy will be calculated using the SM5.0R methodology. The SM5.0R model can predict solvation free energies in water or an organic solvent. The calculation is based entirely on the use of geometry-dependent atomic surface tensions and the exposed solvent accessible surface area using an effective solvent radius of zero. The R in the name represents the "rigid"ness of the model and denotes that the calculation is made from a gas-phase geometry which is not allowed to relax in the presence of the solvent. The SM5.0R model is especially well suited for problems requiring high efficiency because of the size of the system, e. g., protein folding on enzyme-substrate binding, or problems requiring rapid estimations because of the large number of calculations required, e. g., scoring of combinatorial libraries.

****SM5.0R using water as a solvent****

The SM5.0R model predicts aqueous solvation free energies for organic molecules containing H, C, N, O, F, S, Cl, Br, and I. The model was parameterized for water by using a training set containing 248 neutral solutes with a variety of functional groups, and it achieves a mean unsigned error of 0.54 kcal/mol when the model is applied using gas-phase geometries calculated at the Hartree-Fock level with a heteroatom-polarized valence-double-zeta basis

set (HF/MIDI!) and a mean unsigned error of 0.57 kcal/mol when it is applied using gas-phase geometries from Austin Model 1 (AM1).

To use the SM5.0R model with water as a solvent, the keyword SOLVNT=WATER must also be included on the keyword line.

****SM5.0R using a general organic solvent****

The SM5.0R model predicts solvation free energies in organic solvents for organic solute molecules containing H, C, N, O, F, P, S, Cl, Br, and I. The model was parameterized by using a training set containing 227 neutral solutes and 90 organic solvents for a total of 1836 data points. It achieves a mean unsigned error of 0.38 kcal/mol when the model is applied using gas-phase geometries calculated at the Hartree-Fock level with a heteroatom-polarized valence-double-zeta basis set (HF/MIDI!) and a mean unsigned error of 0.39 kcal/mol when it is applied using gas-phase geometries from Austin Model 1 (AM1).

To use the SM5.0R model with organic solvents, the keywords SOLVNT=GENORG, ALPHA=x.xx, BETA=x.xx, FACARB=x.xx, FEHALO=x.xx, GAMMA=x.xx, and IOFR=x.xx.

More details about the SM5.0R model can be obtained from the references listed in Section 1.

3.1.10. Keyword SOLVNT=x

The SOLVNT=x keyword indicates which parameter set will be used in the SM5.0R calculation. Currently, only the options "SOLVNT=WATER" and "SOLVNT=GENORG" are accepted. (Note that there are no spaces in this keyword.) Using "SOLVNT=WATER" with the SM5.0R keyword indicates that an aqueous solvation energy prediction is requested and no further keywords are required. Using the "SOLVNT=GENORG" keyword requests the prediction of a solvation free energy in a general organic solvent which is described by the solvent descriptors specified by the IOFR, ALPHA, BETA, GAMMA, FACARB, and FEHALO keywords. Each of the six solvent descriptor keywords and the SM5.0R keyword must be used with SOLVNT=GENORG.

4. TEST RUN INPUT AND OUTPUT

The keyword and comment lines from the .dat files of the test runs are provided here as a reference. Notice that in the present version of OMNISOL, a .dat file always begins with one or two lines of keywords followed by two comment lines. If the second line of a .dat file begins with an ampersand (&) then this line is assumed to be a second keyword line. Otherwise it is assumed to be the first comment line. In several runs of the test suite, the second comment line is used, and it is blank for all the others. This blank line is, nevertheless, required.

For every test run the .dat file is located in the test directory and the associated .out file as produced from a calculation with a IRIS Indigo2 (R10000 processor) is provided as part of the distribution package in the directory testo. The keywords are explained Section 3.

The data files provided in the distribution package are the files which were run successfully on all the machines on which the code has been tested. Using these data files gave energies that were always within 0.2 kcal/mol (and usually within 0.1 kcal/mol) across all the machines which were tested (see Section 6).

The keyword and comment lines from each test run in the test suite are as follows:

tr01a.dat:

SM5.0R SOLVNT=WATER AMSOLZ
ammonia (aqueous)

tr01n.dat:

SM5.0R AMSOLZ DETAIL
& IOFR=1.4961 ALPHA=0 BETA=0.14 GAMMA=40.2
& FACARB=0.86 FEHALO=0.00 SOLVNT=GENORG
ammonia (solvent: toluene)

tr02a.dat:

SM5.0R SOLVNT=WATER
pentyl ethanoate (aqueous)

tr02n.dat:
SM5.0R AMSOLZ
& IOFR=1.4995 ALPHA=0 BETA=0.16 GAMMA=41.38
& FACARB=0.75 FEHALO=0.00 SOLVNT=GENORG
pentyl ethanoate (solvent : xylene)

tr03a.dat:
SM5.0R SOLVNT=WATER
2-octanone (aqueous)

tr03n.dat:
SM5.0R
& IOFR=1.3878 ALPHA=0 BETA=0 GAMMA=28.28
& FACARB=0.00 FEHALO=0.00 SOLVNT=GENORG
2-octanone (heptane)

tr04a.dat:
SM5.0R SOLVNT=WATER DETAIL
diethyl ether (aqueous)

tr04n.dat:
SM5.0R
& IOFR=1.4459 ALPHA=0.15 BETA=0.02 GAMMA=38.39
& FACARB=0.00 FEHALO=0.75 SOLVNT=GENORG
diethyl ether (solvent : chloroform)

tr05a.dat:
SM5.0R AMSOLZ SOLVNT=WATER
butanoic acid (solvent: water)

tr05n.dat:
SM5.0R AMSOLZ
& IOFR=1.4295 ALPHA=0.37 BETA=0.48 GAMMA=39.01
& FACARB=0.00 FEHALO=0.00 SOLVNT=GENORG
butanoic acid (solvent: octanol)

tr06a.dat:
SM5.0R SOLVNT=WATER
1,2-ethanediol (all trans) (aqueous phase)

tr06n.dat:
SM5.0R
& IOFR=1.4345 ALPHA=0 BETA=0 GAMMA=38.93
& FACARB=0.00 FEHALO=0.00 SOLVNT=GENORG
1,2-ethanediol (all trans) (solvent: hexadecane)

tr07a.dat:
SM5.0R SOLVNT=WATER
allyl vinyl ether (aqueous phase)

tr07n.dat:
SM5.0R
& IOFR=1.5413 ALPHA=0 BETA=0.19 GAMMA=47.74
& FACARB=0.60 FEHALO=0.00 SOLVNT=GENORG
allyl vinyl ether (solvent: tetralin)

tr08a.dat:
SM5.0R SOLVNT=WATER
morpholine (Cs symmetry) (aqueous)

tr08n.dat:
SM5.0R AMSOLZ
& IOFR=1.4102 ALPHA=0 BETA=0 GAMMA=33.64
& FACARB=0.00 FEHALO=0.00 SOLVNT=GENORG
morpholine (Cs symmetry) (decane)
Z matrix adapted from cyclohexane

tr09a.dat:
SM5.0R SOLVNT=WATER
4-pyridone (aqueous phase)
AM1 geometry used

tr09n.dat:
SM5.0R
& IOFR=1.372 ALPHA=0.61 BETA=0.44 GAMMA=39.01
& FACARB=0.00 FEHALO=0.00 SOLVNT=GENORG
4-pyridone (solvent : acetic acid)
AM1 geometry used

tr10a.dat:
SM5.0R SOLVNT=WATER AMSOLZ
Z-1,2-dichloroethylene (C2v symmetry) (aqueous)

tr10n.dat:
SM5.0R
& IOFR=1.3611 ALPHA=0.37 BETA=0.48 GAMMA=31.62
& FACARB=0.00 FEHALO=0.00 SOLVNT=GENORG
Z-1,2-dichloroethylene (C2v symmetry) (solvent : ethanol)

tr11a.dat:
SM5.0R SOLVNT=WATER AMSOLZ
methylcyclohexane (aqueous)

tr11n.dat:
SM5.0R
& IOFR=1.405 ALPHA=0 BETA=0.48 GAMMA=38
& FACARB=0.00 FEHALO=0.00 SOLVNT=GENORG
methylcyclohexane (tetrahydrofuran)

tr12a.dat:
SM5.0R SOLVNT=WATER
1-propanethiol (cyclohexane)

tr12n.dat:
SM5.0R
& IOFR=1.4266 ALPHA=0 BETA=0 GAMMA=35.48
& FACARB=0.00 FEHALO=0.00 SOLVNT=GENORG
1-propanethiol (cyclohexane)

tr13a.dat:
SM5.0R SOLVNT=WATER
1,1,1-trifluoropropan-2-ol (aqueous)

tr13n.dat:
SM5.0R
& IOFR=1.4345 ALPHA=0 BETA=0 GAMMA=38.93
& FACARB=0.00 FEHALO=0.00 SOLVNT=GENORG
1,1,1-trifluoropropan-2-ol (hexadecane)

tr14a.dat:
SM5.0R SOLVNT=WATER AMSOLZ
3-ethyl-2-methoxypyrazine (aqueous)

tr14n.dat:
SM5.0R
& IOFR=1.4295 ALPHA=0.37 BETA=0.48 GAMMA=39.01
& FACARB=0.00 FEHALO=0.00 SOLVNT=GENORG
3-ethyl-2-methoxypyrazine (solvent : octanol)

tr15a.dat:
SM5.0R SOLVNT=WATER
2,2',3'-trichlorobiphenyl (aqueous)

tr15n.dat:
SM5.0R IOFR=1.4459 ALPHA=0.15 BETA=0.02 GAMMA=38.39
& FACARB=0.00 FEHALO=0.75 SOLVNT=GENORG
2,2',3'-trichlorobiphenyl (solvent: chloroform)

tr16n.dat:
SM5.0R SOLVNT=GENORG IOFR=1.5011 ALPHA=0 BETA=0.14 GAMMA=40.62
& FACARB=1.00 FEHALO=0.00
TRIMETHYLPHOSPHATE in benzene

5. OUTPUT

The standard output file of a OMNISOL calculation using the SM5.0R model includes:

- a) A time-date stamp.
- b) An echo of the keywords input on the keyword line.
- c) A summary of the recognized keywords. This can be used to determine whether a keyword was mis-typed and therefore not recognized by the program.
- d) A listing of the Cartesian coordinates.
- e) A matrix containing the interatomic distances.
- f) A table of the atom-by-atom solvent-accessible surface area and the atom-by-atom SM5.0R solvation free energy.
- g) A statement of the total SM5.0R predicted solvation free energy.
- h) The total CPU time used for the calculation.

Additional output can be obtained using the keyword `DETAIL` as described in Section 3.

NOTE: All solvation free energies predicted by the SM5.0R model are standard-state values and are printed in kcal/mol. They correspond to a standard state of 1 mole per liter in both the gas phase and solution.

6. COMPUTERS AND COMPILERS FOR WHICH THE CODE HAS BEEN TESTED

The OMNISOL program is written in FORTRAN 77 with the INCLUDE extension and using lower case letters. The machines and operating systems on which this version of OMNISOL has been tested are listed below:

Version	Machine	Operating system
1.0 & 1.0.1	Cray C90	UNICOS 8.0.3
	IBM RS/6000 model 550	AIX 3.2.5
	SGI Indigo2 R10000	IRIX 6.2
1.1	Altix Itanium 2	RedHat 7.3 Linux
	Compaq ES40 Alpha 500	Tru64 4.0f
	IBM SP Power3	AIX 4.3
	IBM Power4 (Regatta)	AIX 5.1
	Pentium-III (Prestoria)	RedHat 9.0 Linux
	Pentium-4 (Northwood)	WindowsXP
		WinXP/Cygwin
	SGI Octane2 R14000	IRIX 6.5
	Sunblade 2000	Solaris 8
	Apple G4	OS 10.2.8/ Darwin 6.8
2.0	IBM SP Power3	AIX 5.1
	IBM Power4 (Regatta)	AIX 5.2
	Altix Itanium 2	Redhat Linux
	Apple G5	OS 10.4.2/ Darwin 8.2.0

Version	Machine	Compilers tested
1.1	Altix	GNU F77 2.96 (GCC 3.2.2 20000731)
	Compaq	Compaq FORTRAN 5.4-1283
	IBM SP Power3	XL Fortran 7.1
		GNU F77 (GCC 3.3.1 20030804)
	IBM Power4	XL Fortran 7.1
	Pentium-III	GNU F77 3.2.2 (GCC 3.2.2 20030222)
	Pentium-4	MS Fortran PowerStation 4.0
		GNU F77 2.95 (GCC 2.9.5 19990728)
		Cygwin/GNU F77 (GCC 3.3.1)
		SGI Octane2 R14000
		GNU F77 3.0.2 (mips-sgi-irix6.5)
	Sunblade 2000	Forte Developer 7 Fortran 95 7.0
		GNU F77 3.0.3 (sparc-sun-solaris2.8)
	Apple G4	GNU F77 3.1 (GCC 3.1 20020420)
2.0	IBM SP Power3	XL Fortran 9.1
	IBM Power4	XL Fortran 9.1
	Altix	GNU F77 GCC 3.2.3 20030502
	Apple G5	GNU F77 GCC 3.2.3

6.1 Known Issues

To run OMNISOL on some machines requires that the environmental variable LIBPATH is set. (typically to /usr/lib)

6.2. Installing OMNISOL on an Apple machine.

Compiling OMNISOL on an Apple G5 requires that the Apple Developer Toolkit be installed. Also, in most cases the user will need to independently obtain a compiler. The compiler used to test OMNISOL version 2.0 was acquired from <http://fink.sourceforge.net/download/index.php>, and installed using the following commands in Terminal:

- 1.) su (requires that root account has been enabled in NetInfo Manager)
- 2.) source /sw/bin/init.sh
- 3.) apt-get update
- 4.) apt-get upgrade
- 5.) apt-get install g77

With the compiler installed, the OMNISOL source code was then compiled using the following commands:

- 1.) ./omnisol.compile
- 2.) Select "man"
- 3.) Select "Linux"
- 4.) Name the executable file
- 5.) Select "m"
- 6.) make

7. REVISION HISTORY

Version 1.0.1:

1. The parameters for nitrogen-containing solutes in organic solvents were incorrect in version 1.0. The errors have now been corrected.

Version 1.1:

1. OMNISOL now works on Windows 98/NT/2000/XP. The new directory "PC" contains the files needed to compile the code and the script to run the test runs on Windows.
2. The omnisol.compile script now has options to compile on ibm604e (Power3) machines.
3. The omnisol.compile script now has the option to automatically configure and compile the source code.
4. The parameter for phosphorus atom has been added to allow SM5.0R calculations on phosphorus-containing compounds in organic solvents

Version 2.0:

1. A utility program for calculating air-water interface adsorption coefficients with the SM5.0R-Surf model has been added.

8. ACKNOWLEDGMENTS

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End of manual