

## COSMO *therm* Version C2.1 Release 01.07 (November 2007)

New features of this distribution include:

### 1. Improved accuracy and applicability of COSMO *therm* predictions:

- Further improved sets of COSMO *therm* parameters for both high level (BP-TZVP-COSMO) and screening level (BP-SVP-AM1) sigma-profiles were obtained from an enhanced fitting procedure, which includes pure compound and mixture thermodynamic data which is not limited to room temperature. The new COSMO *therm* parameterization sets for BP-TZVP and BP-SVP-AM1 level validated on a massively enlarged set of experimental data, namely non-room-temperature activity coefficients in non-aqueous solvents, Vapor-Liquid Equilibrium (VLE) mixture data (activity coefficient, vapor pressure, gas phase composition, azeotrope data), boiling points and non-room-temperature vapor pressure and enthalpy of vaporization data, solid compound aqueous solubility and activity coefficients of solutes in Ionic Liquid (IL) solvents. The new fitting and validation procedure ensures an improved overall quality of COSMO *therm* predictions and assures a widespread applicability over all areas of organic chemistry and some areas of inorganic chemistry.

### 2. Enhanced and improved COSMO *therm* functionality:

- **PKA:** New pK<sub>A</sub>-LFER parameters for the prediction of acid and base pK<sub>A</sub> in solvent acetonitrile (CH<sub>3</sub>CN) have been added. - An estimated temperature dependency has been introduced into the solid
- **Solubility:** The QSPR free energy of fusion estimate in the solids solubility computation option now allows temperatures other than room temperature. In addition the treatment of conformers in solubility QSPR has been improved in a thermodynamic consistent way.
- **QSPR:** New sigma-moment models for solubility, heat of solvation and partition properties have been added.

### 3. COSMOthermX graphical user interface (GUI):

- Significantly improved and extended graphical user interface with newly written graphics routines that are significantly faster and more reliable. In addition numerous new usage features have been implemented into the GUI:
  - Strongly enhanced functionality: The (nearly) complete functionality of *COSMOtherm* as available in the command line version, now can be toggled and controlled from within the *COSMOthermX* GUI. New control features include "simple mixture" features such as direct input of concentrations, contact probability calculations, similarity calculations and the processing of compound lists (*COSMOtherm* \$DATABASE option).
  - Graphical display of compound geometries and compound charge surfaces has been enhanced to process multi-compounds and conformers.
  - Graphical post-processing of computed thermodynamics has been extended to ternary and n-dimensional "multinary" isobar and isothermal VLE/LLE phase diagrams as well as vapor pressure curves.
  - Rapid 'string' searching, smiles code identifiers and the addition of many synonyms allow for greater ease in the selection of compounds from *COSMObase*.
  - Weight-string and *COSMO*-meta-file editor for the easier set up of advanced polymer, surface and micelle applications.
  - Simplified *COSMObase* (database of *COSMO*-files) installation and new editing function for database entries. Several *COSMO*-file databases can be used from within one compound selection and search window.
  - Improved stability and easier usability plus a simplified installation procedure of the *COSMOthermX* GUI allows for the simple and efficient setup of *COSMOtherm* calculations and the graphical postprocessing of the computed results.
  - In the graphics window, new tool tips allow for easier understanding and creation of plots.
  - Plots now directly can be exported to jpeg graphics format without any loss of graphics quality.
  - All computed tables (graphics tables as well as text files) can be exported to Excel.

#### 4. Improved and simplified COSMO $therm$ input and output:

- All pKA-LFER parameters (acids in water, bases in water, acids in DMSO, acids in acetonitrile, bases in acetonitrile) are now built into the parameter sets and are easily accessible by just one click in the COSMO $thermX$  graphical user interface.
- Output of molar solubility: If the solvent is water, the solubility option will provide the molar [mg/l] solubility as additional output.
- Optional Creation of ion geometry files in contact/cluster option.

## 5. Further extension of *COSMObase*, the database of COSMO-files:

- All of *COSMObase*'s compounds have been re-optimized with the latest Turbomole version TM5.9 and some database entries and/or cosmo-files have been bug-fixed.
- To ensure an optimum prediction quality in *COSMOtherm*, *COSMObase*, compound geometries have been critically reviewed for conformational effects and for a large number of compounds already present in *COSMObase*, additional conformers have been added and/or existing conformers have been replaced by better (lower energy) conformers.
- Currently *COSMObase* holds over 6100 molecular COSMO-files, gas phase energy-files and geometry car-files for high level (BP-TZVP-COSMO) quantum chemistry and over 7000 molecular COSMO-files, gas phase energy-files and geometry car-files for screening level (BP-SVP-AM1) quantum chemistry. This corresponds to over 4100 chemical compounds.
- A large number of compound synonyma and alternative and trivial names has been added to the *COSMObase* database index file, allowing for a simpler identification of a given compound in the database. A unique smiles code (USMI) of the compound geometry has been added to the synonyma of all nonionic compounds in *COSMObase*. Moreover, if available, the Beilstein-, RTECS-, EC-, and Merck-Index code of the compounds has been added to the synonyma.
- Every compound COSMO-file now is accompanied by a vapor pressure and property (`name.vap`) file, holding the compounds CAS registry number and compound experimental data information:
  - Pure compound vapor pressure Wagner or Antoine coefficients, which can be used to obtain the pure compound measured/validated vapor pressure, are available in over 1100 vapor pressure / experimental data property compound vap-files.
  - For more than 3000 of the *COSMObase* compounds experimental boiling points and/or melting points are available in the database index file and the compound vap-files.
  - For over 250 *COSMObase* compounds experimental heat of fusion data (enthalpy of fusion and melting point) and critical point data are available in the compound vap-files.
  - All *COSMObase* molecules are identified with a novel unique code and - if available - by their CAS registry number, .
  - UNIQUAC volume and area coefficients that can be used in the fitting of activity coefficients to the UNIQUAC equation.