



Scientific Computing & Modelling

# ADF COSMO-RS Manual

**ADF Program System  
Release 2014**

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# Introduction

The ADF COSMO-RS (COnductor like Screening MOdel for Realistic Solvents) program is a program that can be used for calculating thermodynamic properties of (mixed) fluids. The COSMO-RS method was developed by Klamt and coworkers [1-3]. On the basis of the framework of COSMO-RS, Lin and Sandler [8] suggested a variation, the COSMO-SAC (where SAC denotes segment activity coefficient) model. There are different implementations of COSMO-RS and COSMO-SAC or derivatives, and different parametrizations. The implementation of COSMO-RS in ADF is described in Ref. [4], which is based on the COSMO-RS method developed by Klamt et al. [2]. The implementation of COSMO-SAC 2013-ADF in ADF is based on the COSMO-SAC model developed by Xiong et al. [9].

[Our COSMO-RS capabilities are summarized on the product page.](#)

With COSMO-RS it is possible to use a thermodynamically consistent combinatorial contribution to the chemical potential as is used in Ref. [3], and a temperature dependent hydrogen bond interaction, also described in Ref. [3]. The parameters in the paper [2] were reparametrized for ADF, see Ref. [4] for details.

The COSMO-SAC 2013-ADF parameters in Ref. [9] were optimized for use with ADF COSMO result files. COSMO-SAC 2013-ADF is an improved COSMO-SAC method compatible to ADF and different than previous COSMO-SAC methods. The main difference that the COSMO-SAC 2013 model includes a dispersion contribution in the mixture interaction. Previous COSMO-SAC methods are described in Refs. [6,7].

The ADF COSMO-RS (and COSMO-SAC) command line program is called *crs*. The main authors of this program are Cory Pye (Saint Mary's University, Halifax NS Canada) and Jaap Louwen (Albemarle Corporation). COSMO-SAC 2013-ADF was implemented in collaboration with R. Xiong and R.I. Burnett (Sandler group, University of Delaware, Newark, USA). Previous COSMO-SAC methods were implemented by Erin McGarrity (TU Delft, the Netherlands). The COSMO-RS GUI *ADFcrs* contains an input builder for COSMO-RS and can visualize results, see the [COSMO-RS GUI tutorials](#) and the [COSMO-RS GUI reference manual](#).

COSMO-RS (and COSMO-SAC) use the intermediate results from quantum mechanical (QM) calculations on individual molecules to predict thermodynamic properties of mixtures of these molecules, for example, solubility. There are a fair number of reports of accurate prediction by COSMO-RS of thermodynamic properties in general in the literature. Many of these have been written by Klamt and co-workers, see Ref. [3] and references therein.

There are also empirical methods like UNIFAC that can predict thermodynamic properties (including the activity coefficients). These methods contain group specific parameters and are parametrized against a large data base. They will often do better than COSMO-RS or COSMO-SAC methods (especially, of course, if the system of interest was part of the data base used for parameter estimation). However, these methods cannot handle every type of molecule. In particular when unusual combinations of functional groups occur (such as in drug molecules), no parametrization is available. COSMO-RS and COSMO-SAC methods, on the other hand, only feature general parameters not specific to chemical groups or functionalities. All that is required is that a quantum mechanical calculation can be done on the molecule. Therefore, COSMO-RS or COSMO-SAC can be a valuable tool for the prediction of chemical engineering thermodynamical properties, like, for example, partial vapor pressures, solubilities, and partition coefficients. An additional advantage of COSMO-RS and COSMO-SAC over empirical methods is that the molecules dissolved may in fact be transition states of a chemical reaction. This follows from the fact that all that is required is that one can do a QM calculation on the solute and QM on a transition state has become standard in the last two decades. This affords a unique opportunity to predict the thermodynamics of a reaction including, for instance, the balance between kinetically and thermodynamically favored reaction pathways as a function of the solvent used.

## Release 2014

The major changes of COSMO-RS 2014 in comparison to COSMO-RS 2013 are described here.

- new [COSMO-SAC 2013-ADF](#): method compatible for use with ADF COSMO result files
  - includes a dispersion contribution in the mixture interaction
  - activity coefficients are calculated according to the COSMO-SAC 2013-ADF method
  - pure compound properties are not calculated according to the COSMO-SAC 2013-ADF method yet

## COSMO-RS GUI

Note that the graphical user interface COSMO-RS GUI enables all users to set up complicated calculations with a few mouse clicks, and provides graphical representations of calculated data fields, see the [COSMO-RS GUI tutorials](#).

# COSMO-RS and COSMO-SAC

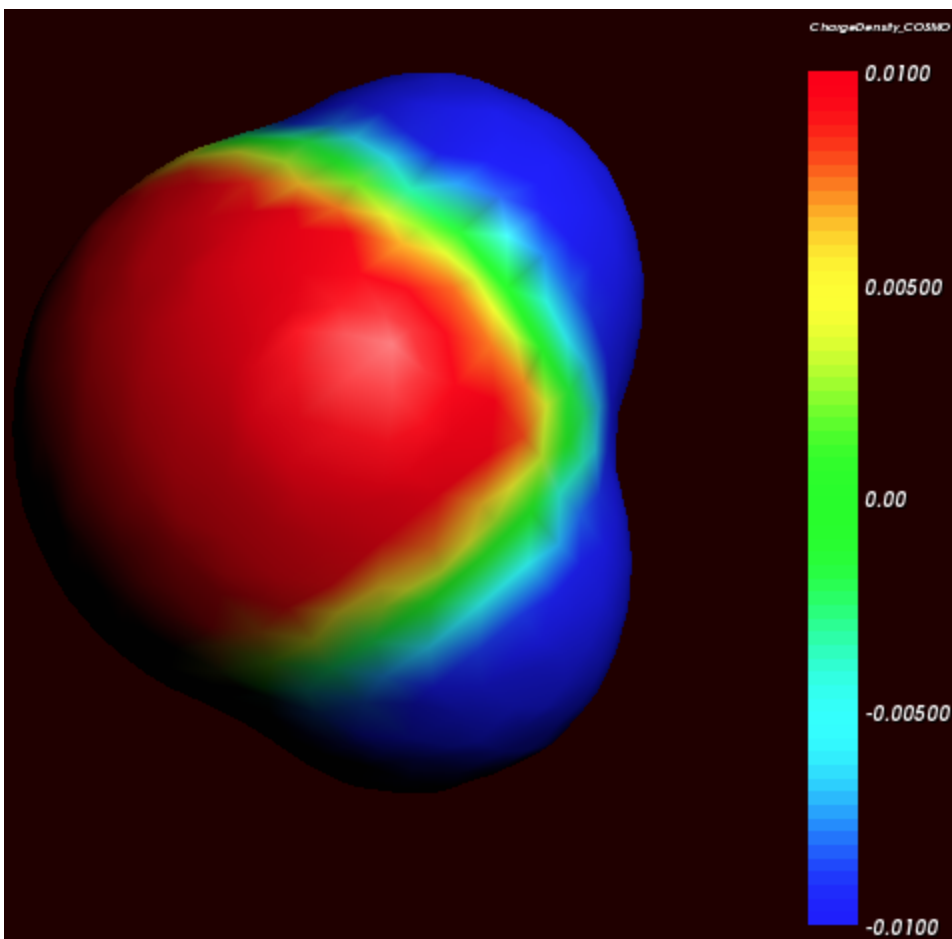
## COSMO-RS

Below some of the COSMO-RS theory is explained, but a more complete description can be found in Refs.[2] and [3].

Although in principle all of chemistry can be predicted by appropriate solutions of the Schrödinger Equation, in practice due to the extreme mathematical complexity of doing so only the smallest systems can be computed at an accuracy rivaling that of the most accurate experiments. However, with suitable approximations, for isolated molecules of up to a few hundred atoms these days quite reasonable results can be obtained. Of course, this means that direct computation of thermodynamic properties is out of reach. Thermodynamic properties can only be computed as an average over a large number of configurations of a large number of molecules. To address this, people have typically resorted to so-called Molecular Dynamics (MD) or Monte Carlo (MC) methods where configurations are generated either by numerically simulating the atomic motions over discrete time steps or by random generation, in either case using empirical molecular models parametrized against quantum mechanical calculations and experimental data to compute energies. However, even these approaches often fall short in generating sufficiently large ensembles, and there is little chance of that situation improving dramatically in the near future.

Around 1995, Andreas Klamt, then working for Bayer, hit upon an approach that made it possible to compute the details of molecules quantum mechanically and subsequently use these details in an approximate statistical mechanics procedure [1]. This approach is called COSMO-RS (COnductor like Screening MOdel for Realistic Solvents) and has proven to be quite powerful. It may currently be the best link between the world of chemical quantum mechanics and engineering thermodynamics.

Thermodynamic reference states can be chosen arbitrarily. They do not even have to be physically realizable, as long as it is consistently used. We are at liberty to choose as reference state a molecule embedded in a perfect conductor, that is a material with an infinitely large dielectric constant ('the perfectly screened state'). Suppose a molecule A resides in a molecule shaped cavity. Everywhere outside of this cavity is conductor material. Although it would be hard to realize this in practice, it is relatively easy to do quantum mechanical calculations on this hypothetical state. Since the molecule will in general have a charge distribution and therefore possess an electric field, it will polarize the embedding medium. That will result in another electric field, given by a charge distribution on the surface of the molecule shaped cavity. This charge distribution is generated by the quantum mechanical calculations, for example with ADF if one uses COSMO. From now on the surface of the molecule shaped cavity will be called molecular surface, and the volume of the molecule shaped cavity will be called molecular volume.



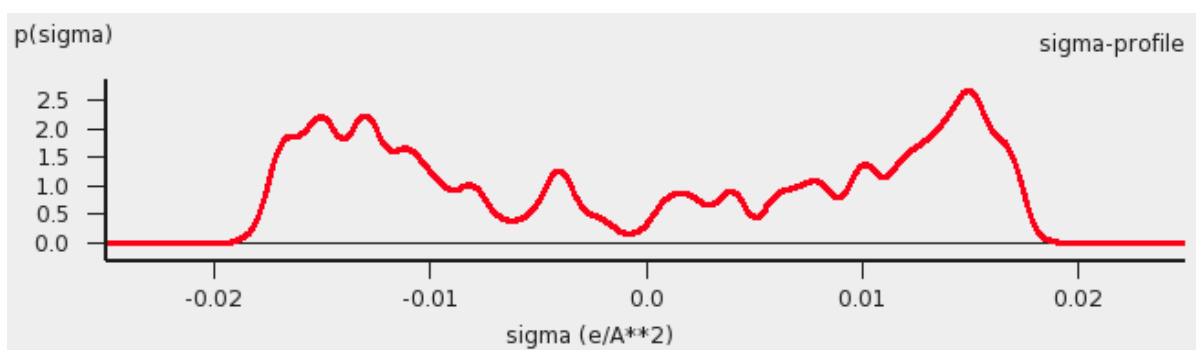
*Cosmo charge density on the COSMO surface of water (picture made with ADFview)*

Although the actual charge distribution on the molecular surface will be highly detailed, let us for the moment consider the molecular surface as consisting of segments with a constant charge density (i.e. the detailed charge distribution averaged over segments). Now instead of the single molecule A consider, as an arbitrary example, a fluid consisting of three types of molecules: A, B and C. In a fluid not too close to the critical temperature, the molecular surfaces present in the fluid will all be in close contact. That means that the segments of constant density introduced above are in close contact.

We now compare our molecule A in the fluid with our chosen reference state. Any segment of the molecular surface with a charge density of  $\sigma_i$  will be aligned with a segment with charge density  $\sigma_j$  of another molecule. If the two charge densities happen to be opposite (i.e.  $\sigma_i + \sigma_j = 0$ ) the charges required for achieving the perfectly screened state will vanish. However, this will not happen too often and in general an excess charge density is left of  $\sigma_i + \sigma_j$  between the two segments. From electrostatic theory it follows that this introduces an energy penalty proportional to the segment size and  $(\sigma_i + \sigma_j)^2$ . In principle this gives a way to compute the chemical potential of component A, by going over all possible conformations of a large number of molecules A, B and C (in their proper molar fractions) and do computations on the statistical ensemble. However, in practice that would be similar to doing Molecular Dynamics calculations using empirical structure models and about as computationally prohibitive. Instead, an approximation can be made that is not easily justified a priori and must be judged by the results of subsequent simulations. This assumption is that all segments in the fluid are able to make contact independent of one another. In a way it can be said, that the segments are cut loose from the original (rigid) molecular surfaces.

As one would guess, the approximation of independent segments makes the mathematics of computing ensemble properties quite tractable. In fact, computing the chemical potential of component A (or B or C) in

the mixture by means of the COSMO-RS and related methods takes in the order of seconds on a normal PC (given the results of quantum mechanical calculations that may have taken days, of course). Note that the molecular surface around the molecule is divided rather arbitrarily in segments and that the assumption was that the segment of one molecule will overlap perfectly with that of another. How can this be true? The answer is that one can split up the molecular surface into segments in an infinite number of ways. However, the molecules in a fluid are always in contact with another. At any given time, molecule A will be in contact with a number of other molecules and share patches of, for example, 7 square Angstroms of its surface with each of the surrounding molecules. At that particular time, the segments will be those patches. A split second later, of course, there will be a different set of segments. That is not a problem. One needs to do statistical mechanics with charged segments for which one needs to know how many 7 square Angstrom segments a particular molecule brings into the fluid and the probability of any segment having an average charge density  $\sigma$  (for all values of  $\sigma$ ). Both can be computed from the results of the quantum mechanical calculation on the molecule in the perfect conductor. Just to get a flavor, in the figure below the so-called  $\sigma$ -profile of water is given. These are the statistical distributions of possible segments over charge densities multiplied by the surface area of the molecular volume. The  $\sigma$ -profile relates to the detailed charge distribution on the molecular surface.



*$\sigma$ -profile of water (picture made with the CRS-GUI), smoothed curve, Delley COSMO surface construction*

In principle vapor pressures of pure liquids can be computed directly with COSMO-RS. COSMO-RS calculations yield the chemical potential of a component in a liquid with respect to the perfectly screened reference state. It is easy to compute the energy difference between the reference state and the gas phase by doing an additional quantum mechanical calculation (of the isolated molecule). However, often experimental vapor pressures for the pure liquid are known. Using such experimental data for pure liquids can help in predicting the correct partial vapor pressures in a mixture.

## COSMO-RS combinatorial term

In Ref.[2] a thermodynamically inconsistent combinatorial contribution  $\mu_i^{\text{comb}}$  to the chemical potential was used:

$$\mu_i^{\text{comb}} = -\lambda RT \ln (q_{\text{av}}/\text{Angstrom}^2)$$

$$q_{\text{av}} = \sum_i x_i q_i$$

In this equation  $q_i$  is the surface area of the molecular volume of compound  $i$ ,  $x_i$  is the molar fraction of compound  $i$  in the solution, and  $\lambda$  is a COSMO-RS parameter.

The importance of using a thermodynamically consistent combinatorial contribution is discussed in Ref. [3]. In the ADF COSMO-RS program it is possible to use a thermodynamically consistent combinatorial contribution of the form (Equation C.4 of Ref.[3], with  $\lambda_0=\lambda_1=\lambda_2=\lambda$ ):

$$\mu_i^{\text{comb}} = \lambda RT (1 - r_i/r_{\text{av}} + \ln(r_i/r_{\text{av}}) + 1 - q_i/q_{\text{av}} - \ln(q_{\text{av}}/\text{Angstrom}^2))$$

$$r_{\text{av}} = \sum_i x_i r_i$$

In this equation  $r_i$  is the molecular volume of compound  $i$ . In the ADF COSMO-RS program this combinatorial term is used by default, see also Ref. [4].

## Fast approximation for COSMO-RS calculations

In the 1998 COSMO-RS model each segment of the molecular surface has a charge density of  $\sigma_v$ , but also a second charge density  $\sigma_v^\perp$ , which is a descriptor for the correlation between the charge density on the segment with its surrounding. In the original ADF COSMO-RS implementation this was treated as a 2-dimensional problem, in the fast approximation this is effectively reduced to 1-dimension. Starting from COSMO-RS 2010 this fast approximation is now the default. This approximation reduces the computation time, especially in cases of more than 1 compound.

## Temperature dependent hydrogen bond interaction

In Ref.[3] a temperature dependent hydrogen bond interaction is suggested, which is used by default in the ADF COSMO-RS program. The temperature dependence (Equation 6.2 of Ref.[3]) is of the form:

$$\text{term}(T) = T \ln[1 + \exp(20 \text{ kJ/mol}/RT)/200]$$

$$f_{\text{hb}}(T) = \text{term}(T)/\text{term}(298.15 \text{ K})$$

Note that here the correct formula is used with a plus sign before 20 kJ/mol (there is a sign error in Equation 6.2 of Ref.[3], see online 'List of Errata in the COSMO-RS book' by Andreas Klamt), such that this factor goes to zero for large  $T$ . In this equation  $R$  is the gas constant and  $T$  the temperature (in Kelvin). In the ADF COSMO-RS program the hydrogen bond interaction of Ref.[2] is multiplied by this factor  $f_{\text{hb}}(T)$  to make the hydrogen bond interaction temperature dependent.

## COSMO-SAC 2013-ADF

On the basis of the framework of COSMO-RS, Lin and Sandler [8] suggested a variation, the COSMO-SAC (where SAC denotes segment activity coefficient) model by invoking a necessary thermodynamic consistency criterion. Although there are differences, COSMO-RS and COSMO-SAC share some similarities. Later improvements of COSMO-SAC appeared, like in Refs. [6,7,9]. The COSMO-SAC 2013-ADF method used in ADF is the one developed by Xiong et al., which is described in detail in Ref. [9]. The COSMO-SAC 2013-ADF parameters in Ref. [9] were optimized for use with ADF COSMO result files. COSMO-SAC 2013-ADF is an improved COSMO-SAC method compatible to ADF and different than previous COSMO-SAC methods. The main difference compared to previous COSMO-SAC methods is that the COSMO-SAC 2013 model includes a dispersion contribution in the mixture interaction.

The ADF COSMO-RS program can calculate activity coefficients using the COSMO-SAC 2013-ADF model, based on Ref. [9]. Like in the COSMO-RS method, pure compound vapor pressures can be given as input, for example, if experimental values are available. If these values are not specified then the pure compound vapor pressure will not be calculated according to the COSMO-SAC 2013-ADF model, because this part of the COSMO-SAC 2013-ADF has not been implemented in ADF. However, in that case pure compound vapor pressures will be approximated using a method similar as in the COSMO-RS method. Thus only the activity coefficients in the ADF implementation are calculated according to the COSMO-SAC 2013-ADF method. It is also possible to use some earlier COSMO-SAC methods [6,7], but note that the parameters in those methods were not optimized for use with ADF COSMO result files.



The COSMO-SAC 2013 model includes a dispersion contribution in the mixture interaction. This dispersion contribution is a complicated expression which also depends on the liquid molar volume of the pure compounds and on the molar volume of the mixture. The molar volume of the mixture is calculated from the pure compound liquid molar volumes assuming ideal mixing. In the input for the ADF COSMO-RS program one include for each compound the experimental pure compound liquid density (kg/L), from which the program can calculate the pure compound liquid molar volumes. If this density is not given the pure compound liquid molar volume will be calculated from its COSMO volume. Note that in the calculations with the COSMO-SAC 2013-ADF model in Ref. [9] often experimental pure compound liquid molar volumes were used.

## Calculation of properties

The COSMO-RS method allows to calculate the (pseudo-)chemical potential of a compound in the liquid phase, as well as in the gas phase, see the the COSMO-RS theory that was discussed before and Ref.[2]. In the ADF COSMO-RS implementation the following equations were used to calculate properties using these chemical potentials.

$$\sum_i x_i = \sum_i y_i^{\text{vapor}} = \sum_i w_i = 1$$

$$w_i = x_i M_i^{\text{pure}} / M^{\text{ave}}$$

$$M^{\text{ave}} = \sum_i x_i M_i^{\text{pure}}$$

$$p_i^{\text{pure}} = \exp \{(\mu_i^{\text{pure}} - \mu_i^{\text{gas}}) / RT\}$$

$$p_i^{\text{vapor}} = x_i \exp \{(\mu_i^{\text{solv}} - \mu_i^{\text{gas}}) / RT\}$$

$$p^{\text{vapor}} = \sum_i p_i^{\text{vapor}}$$

$$y_i^{\text{vapor}} = p_i^{\text{vapor}} / p^{\text{vapor}}$$

$$Y_i = \exp \{(\mu_i^{\text{solv}} - \mu_i^{\text{pure}}) / RT\}$$

$$a_i = Y_i x_i$$

$$G^E = \sum_i x_i (\mu_i^{\text{solv}} - \mu_i^{\text{pure}})$$

$$H^E = -RT^2 \partial \{G^E / RT\} / \partial T$$

$$G^E = H^E - TS^E$$

$$\Delta_{\text{vap}}H = RT^2 / p^{\text{vapor}} \partial \{p^{\text{vapor}}\} / \partial T$$

$$k_H = 1 / V_{\text{solvent}} \exp \{(\mu_i^{\text{gas}} - \mu_i^{\text{solv}}) / RT\}$$

$$k_H^{\text{cc}} = k_H RT$$

$$k_{H,\text{inv}}^{\text{px}} = 1 / (k_H V_{\text{solvent}}) = Y_i p_i^{\text{pure}}$$

$$x_i^{\text{SOL}} = 1 / Y_i \quad (T > T_m)$$

$$x_i^{\text{SOL}} = 1 / Y_i \exp \{ \Delta H_{\text{fus}} (1/T_m - 1/T) / R - \Delta C_p (\ln(T_m/T) - T_m/T + 1) / R \} \quad (T < T_m)$$

$$\Delta G_{\text{solv}}^{\text{liq-solv}} = \mu_i^{\text{solv}} - \mu_i^{\text{pure}}$$

$$\Delta G_{\text{solv}}^{\text{gas-solv}} = \mu_i^{\text{solv}} - \mu_i^{\text{gas}} + RT \ln(V_{\text{solvent}} / V_{\text{gas}})$$

$$\log_{10} P_{\text{solv1/solv2}} = 1 / \ln(10) (\mu_i^{\text{solv2}} - \mu_i^{\text{solv1}}) / RT + \log_{10}(V_{\text{solv2}} / V_{\text{solv1}})$$

$$1 / \text{LFL}_{\text{mix}} = \sum_i (y_i^{\text{vapor}} / \text{LFL}_i)$$

The above equations are not always exact, some assume ideal gas behavior, for example.

The molar fraction  $x_i$  of each compound  $i$  of the solvent should add up to 1.

With the COSMO-RS method it is possible to predict vapor pressures. In the COSMO-RS model the free energy difference between the chemical potential in the gas phase (ideal gas with a reference state of 1 bar) and the chemical potential of the liquid phase has been defined in such a way that the equation:  $p_i^{\text{pure}} = \exp\{(\mu_i^{\text{pure}} - \mu_i^{\text{gas}})/RT\}$ , will give the pressure in units of bar. It is also possible to use experimental vapor pressures of pure compounds as input data for the calculation. This may increase the accuracy of the calculated vapor pressures in a mixture, for example.

In the COSMO-RS method the volume of 1 molecule in the liquid phase is approximated with the volume of the molecule shaped cavity, that is used in the COSMO calculations. In this way it is possible to calculate the volume of 1 mole of solvent molecules in the liquid phase. However, for properties that depend on such volumes, one can also use (related) experimental data as input data for the calculation.

The calculation of the boiling temperature of a solvent is performed with an iterative method. The temperature is varied until the calculated vapor pressure is within a certain threshold of the desired pressure.

Also the calculation of solubility of compound  $i$  is performed with an iterative method, since the activity coefficient  $\gamma_i$  depends on the molar fraction of this compound. The COSMO-RS method does not predict  $\Delta H_{\text{fus}}$ ,  $\Delta C_p$ , or  $T_m$ . These can be given as input data for the calculation of solubility calculations of solid compounds.

Starting from ADF2012 the Gibbs-Helmholtz equation is used to calculate the excess enthalpy of a mixture. Previously it was estimated using the misfit and hydrogen bonding energy of the mixture and its pure compounds.

Quantity	Meaning
R	Gas constant
T	Temperature
$x_i$	The molar fraction of compound $i$ in a liquid solution
$y_i^{\text{vapor}}$	The molar fraction of compound $i$ in the gas phase
$w_i$	The mass fraction of compound $i$ in a liquid solution
$M_i^{\text{pure}}$	The molar mass of the pure compound $i$
$M^{\text{ave}}$	The average molar mass of the mixture
$\gamma_i$	Activity coefficient of compound $i$ in a liquid solution
$a_i$	Activity of compound $i$ in a liquid solution
$p_i^{\text{pure}}$	The vapor pressure of the pure compound $i$
$p_i^{\text{vapor}}$	The partial vapor pressure of compound $i$
$p^{\text{vapor}}$	The total vapor pressure
$\mu_i^{\text{gas}}$	The pseudochemical potential of the pure compound $i$ in the gas phase
$\mu_i^{\text{pure}}$	The pseudochemical potential of the pure compound $i$ in the liquid phase
$\mu_i^{\text{solv}}$	The pseudochemical potential of compound $i$ in a liquid solution
$G^E$	The excess Gibbs free energy
$H^E$	The excess enthalpy, Gibbs-Helmholtz equation
$\Delta_{\text{vap}}H$	The enthalpy of vaporization, Clausius-Clapeyron equation
$E_i^{\text{HB pure}}$	The hydrogen bond energy of the pure compound $i$ in the liquid phase, see Ref.[2]
$E_i^{\text{HB}}$	The partial hydrogen bond energy of compound $i$ in a liquid solution

$E_i^{\text{misfit pure}}$	The misfit energy of the pure compound $i$ in the liquid phase, see Ref.[2]
$E_i^{\text{misfit}}$	The partial misfit energy of compound $i$ in a liquid solution
$\Delta G_{\text{solv}}^{\text{liq-solv}}$	The solvation Gibbs free energy from the pure compound liquid phase to the solvated phase
$\Delta G_{\text{solv}}^{\text{gas-solv}}$	The solvation Gibbs free energy from the pure compound gas phase to the solvated phase, with a reference state of 1 mol/L in both phases
$k_H$	Henry's law constant: ratio between the liquid phase concentration of a compound and its partial vapor pressure in the gas phase
$k_H^{\text{cc}}$	dimensionless Henry's law constant: ratio between the liquid phase concentration of a compound and its gas phase concentration
$k_{H,\text{inv}}^{\text{px}}$	Henry's law constant, representing the volatility instead of the solubility, ratio between the partial vapor pressure of a compound in the gas phase and the molar fraction in the liquid phase
$V_{\text{solvent}}$	Volume of 1 mole of solvent molecules in the liquid phase
$V_{\text{gas}}$	Volume of 1 mole of molecules in the gas phase (at 1 atm, ideal gas)
$x_i^{\text{SOL}}$	Solubility of compound $i$ in a solvent (molar fraction)
$\Delta H_{\text{fus}}$	The enthalpy of fusion of compound $i$
$\Delta C_p$	The $\Delta$ heat capacity of fusion of compound $i$
$T_m$	The melting temperature of compound $i$
$\log_{10} P_{\text{solv1/solv2}}$	The logarithm of the partition coefficient $P$ , which is the ratio of the concentrations of a compound in two immiscible solvents, solvent 1 and solvent 2
$\text{LFL}_i$	The flash point (lower flammable limit, LFL) of compound $i$
$\text{LFL}_{\text{mix}}$	The flash point (lower flammable limit, LFL) of a mixture, Le Chatelier's mixing rule

See also the COSMO-RS GUI tutorial for the calculation of the following properties:

- solvent vapor pressure [1,2]
- boiling point of a solvent [1]
- partition coefficients (log  $P$ ) [1,2], Octanol-Water partition coefficients (log  $P_{\text{OW}}$ ) [1]
- activity coefficients [1,2], solvation free energies [1], Henry's law constants [1]
- solubility [1,2]
- vapor-liquid diagram binary mixture (VLE/LLE) [1,2]
- $pK_a$  values [1]

## COSMO result files

COSMO-RS needs as input for the calculation so called COSMO result files for each compound, which are results of quantum mechanical calculation using COSMO. In ADF such a COSMO result file is called a TAPE21 (.t21) file or a COSKF file (.coskf). With MOPAC such a COSMO result file is a .cos file, which can be converted to a COSKF file. In other programs such a file can be a .cosmo file. ADF has a database of .coskf files, the COSMO-RS compound database [ADFCRS-2010](#). At <http://www.design.che.vt.edu/VT-Databases.html> a database of .cosmo files can be found, which were made with a different program. Note that the optimal COSMO-RS parameters may depend on the program chosen.

## ADF COSMO calculation

### ADF COSMO settings

Here it is described briefly how to make COSMO result files consistent with the way they were made for the ADF parametrization of COSMO-RS to ensure full parameter applicability. First a gas phase geometry optimization should be performed with ADF, with a small core TZP basis set, the Becke-Perdew functional, the relativistic scalar ZORA method, and an integration accuracy of 6:

```
BASIS
type TZP
core Small
I ZORA/TZ2P/I.4p
END
XC
GGA Becke Perdew
END
INTEGRATION 6 6 6
relativistic scalar zora
```

For heavier elements than krypton ( $Z>36$ ), like iodine, a small core TZ2P basis set is required. The resulting TAPE21 of the molecule (rename it compound\_gasphase.t21) is used as a restart file in the COSMO calculation. The ADF COSMO calculation is performed with the following settings:

```
SYMMETRY NOSYM
SOLVATION
  Surf Delley
  Solvent name=CRS emp=0.0 cav0=0.0 cav1=0.0
  Charged method=CONJ corr
  C-Mat EXACT
  SCF VAR ALL
RADIO
  H 1.30
  C 2.00
  N 1.83
  O 1.72
  F 1.72
  Si 2.48
  P 2.13
  S 2.16
  Cl 2.05
  Br 2.16
  I 2.32
SubEnd
```

```

END
XC
GGA Becke Perdew
END
INTEGRATION 6 6 6
relativistic scalar zora
RESTART compound_gasphase.t21

```

In this COSMO calculation the non-default Delley type of cavity construction is chosen (See Ref.[5] for details on the Delley surface construction). The name of the solvent is CRS, which sets the dielectric constant to infinite and sets the radius of the probing sphere to determine the solvent excluded part of the surface to 1.3 Angstrom. In the Radii subblock key the Klamt atomic cavity radii are chosen. The parameters `emp`, `cav0`, and `cav1` are zero. The `corr` option to the CHARGED subkey constrains the computed solvent surface charges to add up to the negative of the molecular charge. Specifying `exact` for the C-MAT subkey causes ADF to compute straightforwardly the Coulomb potential due to the charge  $q$  in each point of the molecular numerical integration grid and integrate against the electronic charge density. This is, in principle, exact but may have inaccuracies when the numerical integration points are very close to the positions of a charge  $q$ . To remedy this, starting from ADF2010 the electrostatic potential is damped in case of (very) close lying numerical integration points and COSMO surface points. The numerical stability of the results compare to those of ADF2009 was increased as a result of this. Specifying `exact` for the C-MAT subkey also requires that the ADF calculation uses SYMMETRY NOSYM.

The resulting TAPE21 (rename it `compound.t21`) of the COSMO calculation is a COSMO result file.

In a COSMO-RS calculation only the 'COSMO' part of this file is needed. One can make a `kf` file `compound.coskf`, which only consists of the section 'COSMO' if one does:

```

| $ADFBIN/cpkf compound.t21 compound.coskf "COSMO"

```

The file `compound.coskf` should not exist before this command is given. Note that such a `.coskf` file is not a complete TAPE21 anymore. For example, only the COSMO surface can be viewed with ADFview. It is useful mostly for COSMO-RS calculations.

### Links

COSMO-RS GUI tutorial: COSMO result files [1]

## Accuracy

Several parameters in the COSMO calculation can influence the accuracy of the result of the quantum mechanical calculation. Some of these parameters will be discussed. Note that if one chooses different parameters in the COSMO calculation one may also have to reparametrize the ADF COSMO-RS parameters. A list of some of the ADF COSMO parameters.

- XC functional
- basis set
- fit set
- atomic cavity radii and radius of the probing sphere
- cavity construction
- geometry

The atomic cavity radii and the radius of the probing sphere are the same as in Ref. [2], which describes the COSMO-RS method developed by Klamt et al., which is implemented in ADF. The Becke Perdew functional is relatively good for weakly bound systems, but may not be so good in other cases. The basis set TZP is a compromise basis set. For heavier elements than krypton ( $Z > 36$ ), like iodine, a TZ2P basis set is required, including the relativistic scalar ZORA method. Since the relativistic method hardly cost extra time compared to a non-relativistic method, the scalar relativistic scalar ZORA method is recommended to be used also for

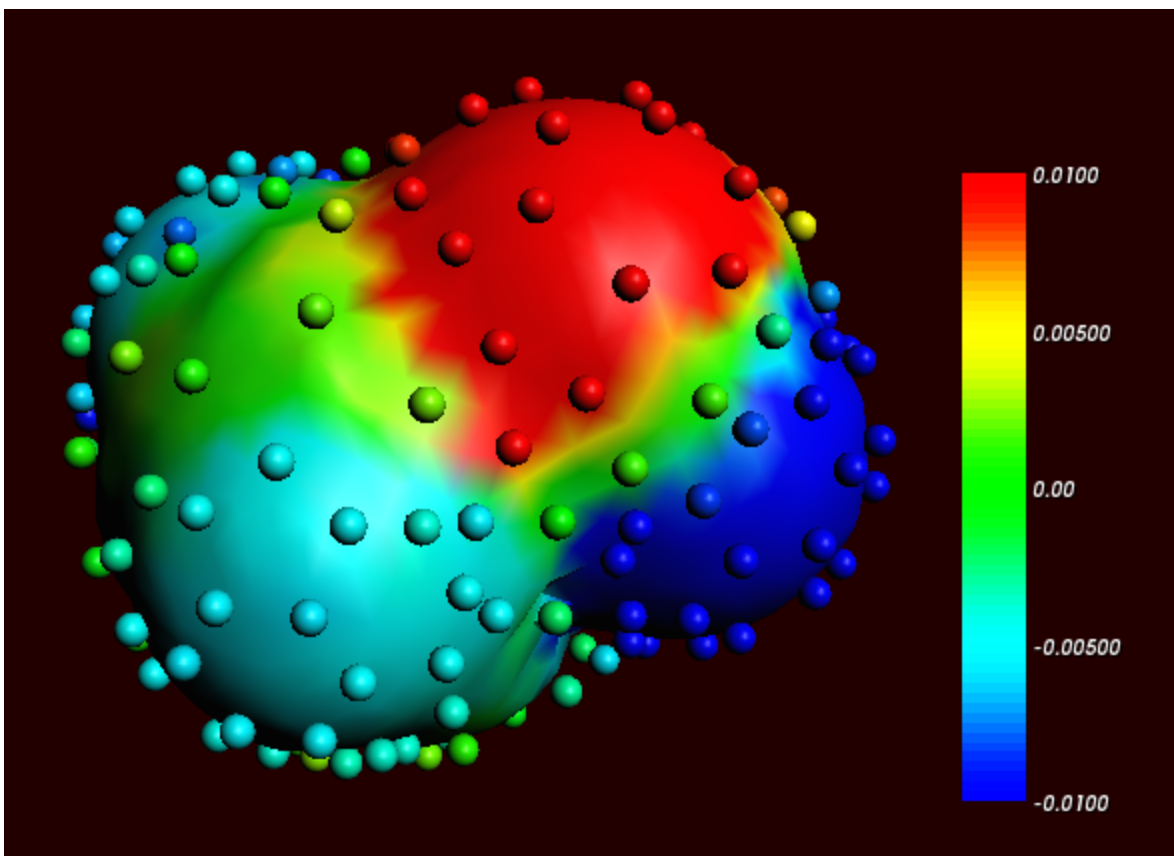
light elements. The Delley type of cavity construction in ADF can give a large number of COSMO points. The XC functional, basis set, and cavity construction chosen in the ADF COSMO calculation have a similar accuracy as those that were used in Ref. [2]. Note that they are not exactly the same as were used in Ref. [2], since in that paper a different quantum mechanical program was used.

In the parametrization for ADF the same geometry was used for the gas phase and the COSMO calculation, which is different than in Ref. [2]. It depends on the actual solvent if reoptimizing the molecule in the COSMO calculation may give better results. Note that the dielectric medium used in the COSMO model has an infinite dielectric constant in the COSMO-RS model. Thus a geometry optimization of the molecule in the COSMO calculation might be more appropriate for a molecule dissolved in water than for a molecule dissolved in n-hexane.

The fit set in ADF is not always able to describe the Coulomb potential accurately at each of the COSMO surface points. In regular ADF calculations this problem is not apparent since the numerical errors in the integrals computed in the vicinity of the COSMO surface have little impact. However, in COSMO calculations this may have some effect. This is why the option `C-Mat_exact` was selected above, instead of the default `C-Mat_pot` option. Another possibility is to add more fit functions, for example, using the `ADDDIFFUSEFITFUNCTIONS` key in the input for the `adf` calculation.

## Cavity construction

The `Esurf` type of cavity construction in ADF with default settings does not give a large number of COSMO points. Therefore it is recommended to use the so called Delley type of cavity construction (Ref.[5]), which allows one to construct a surface which has many more points. The `Esurf` type of cavity construction also allows many more points if one sets the option `NFDiv` of the subkey `DIV` of the key `SOLVENT` to a larger value than the default value of 1. This will not be discussed here further. In ADF2010 the numerical stability of the Delley surface has been improved, by merging close lying COSMO surface points, and removing COSMO surface points with a small surface area. A figure of a COSMO surface with the `Esurf` type of cavity construction with default settings is given below. In this figure the small spheres represent the COSMO surface points that are used for the construction of the COSMO surface. The red part represents positive COSMO charge density, the blue part negative COSMO charge density (the coloring scheme is chosen to match the one by Klamt):



*Cosmo charge density on the COSMO surface of methanol, Esurf surface (picture made with ADFview)*

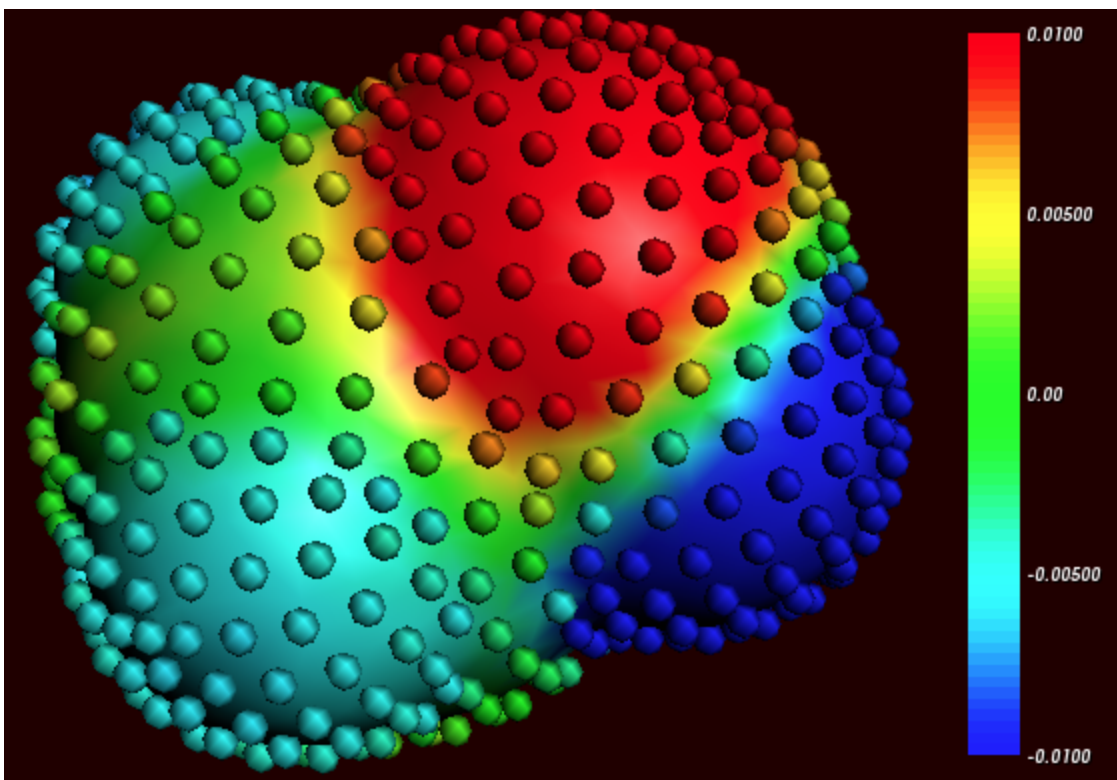
One can construct a surface which has many more points using a so called Delley surface. For the subkey SURF of the key SOLVENT one can choose `delley`. The subkey DIV of the key SOLVENT has extra options `leb1` (default value 23), `leb2` (default value 29), and `rleb` (default value 1.5 Angstrom). If the cavity radius of an atom is lower than `rleb` use `leb1`, otherwise use `leb2`. These values can be changed: using a higher value for `leb1` and `leb2` gives more surface points (maximal value `leb1`, `leb2` is 29). A value of 23 means 194 surface points in case of a single atom, and 29 means 302 surface points in case of a single atom. Typically one could use `leb1` for the surface point of H, and `leb2` for the surface points of other elements.

The next figure is made with the following (default for the Delley surface) settings:

```

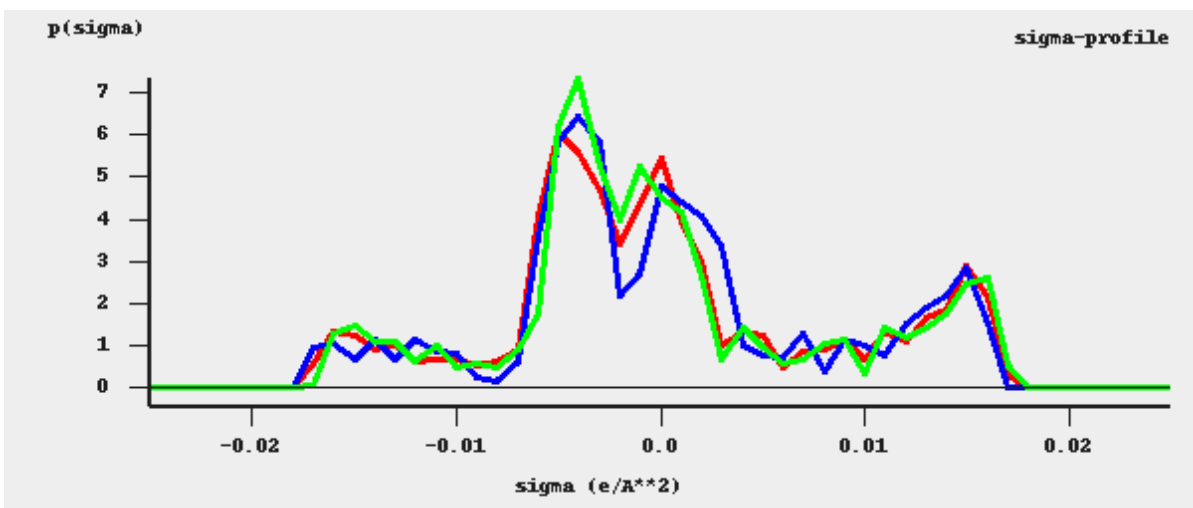
SOLVATION
  SURF Delley
  DIV leb1=23 leb2=29 rleb=1.5
  ....
END

```



Cosmo charge density on the COSMO surface of methanol, Delley surface (picture made with ADFview)

The different ways of constructing the cavity has some consequences for the  $\sigma$ -profile of methanol, see the figure below:



$\sigma$ -profiles of methanol (picture made with the CRS-GUI)

In this picture the blue line is the  $\sigma$ -profile with the Esurf type of construction, the red line is that with the Delley type of construction with many surface points. For comparison, the green line is the  $\sigma$ -profile of methanol if a large QZ4P basis set is used, again with the Delley type of construction with many surface points.



## COSMO-RS Database ADFCRS-2010

The COSMO-RS Database ADFCRS-2010 contains 1892 compounds, mostly solvents and small molecules. This database consists of ADF COSMO result (.coskf) files, which are results of ADF quantum mechanical calculations using COSMO, with settings suitable for use in our COSMO-RS module. The geometries have been optimized with ADF. This database makes the COSMO-RS functionality much easier and faster (the time-consuming DFT step is already done ..) to use. Follow the [COSMO-RS GUI tutorials](#) for more information on how to download and install this database.

The starting point for this database was a database of structures made by Prof. Sandler's group at the University of Delaware. The work of the Sandler group is based in part on earlier work by the group of Prof. Liu at Virginia Technical University, reported in these papers:

Mullins, E.; Oldland, R.; Liu, Y.A.; Wang, S.; Sandler, S.I.; Chen, C.-C.; Zwolak, M.; Seavey, K.C. *Sigma-Profile Database for Using COSMO-Based Thermodynamic Methods*. *Ind. Eng. Chem. Res.* 2006, **45** (12), 4389-4415.

Mullins, E.; Liu, Y.A.; Ghaderi, A.; Fast, S.D. *Sigma Profile Database for Predicting Solid Solubility in Pure and Mixed Solvent Mixtures for Organic Pharmacological Compounds with COSMO-Based Thermodynamic Methods*. *Ind. Eng. Chem. Res.* 2008, **47** (5), 1707-1725.

Phillips, K.L.; Sandler, S.I.; Greene, R.W.; Di Toro, D.M. *Quantum Mechanical Predictions of the Henry's Law Constants and Their Temperature Dependence for the 209 Polychlorinated Biphenyl Congeners*. *Environ. Sci. Technol.* 2008, **42** (22), 8412-8418.

All structures in the database ADFCRS-2010 differ from those in the papers above, as they are the result of ADF geometry optimizations.

The database contains CAS Registry Numbers. CAS Registry Number is a Registered Trademark of the American Chemical Society.

## MOPAC COSMO calculation

Here it is described briefly how to make MOPAC COSMO result files.

The simplest way is to use ADFinput. Draw the molecule using ADFinput, and save the .adf file. Select **Right Panel** → **MOPAC** → **Solvation method** → **COSMO-CRS**. Press Run to run the MOPAC calculation. A .coskf file will be saved that can be used as input in COSMO-RS calculations.

Technically ADFinput will add some keywords to the input for MOPAC (see also <http://www.openmopac.net>). The main input keys for MOPAC that are used are:

```
| PM6 EPS=9999.9 RSOLV=1.3 COSWRT NSPA=362
```

The use of COSWRT makes MOPAC create a .cos file, which is converted to a .coskf file by \$ADFBIN/cosmo2kf:

```
| cosmo2kf file.cos file.coskf
```

Note that this is automatically done if one uses ADFinput.

Compared to the default ADF COSMO-RS values a few [COSMO-RS parameters](#) were reoptimized for MOPAC PM6 COSMO result files to improve the calculation of a number of partition coefficients, when compared to experimental values. Note that MOPAC is a semi-empirical quantum chemistry program, whereas ADF is based on density functional theory (DFT). Thus the MOPAC COSMO result files will not be of the same quality as the ADF COSMO result files.

# The COSMO-RS program

The ADF COSMO-RS command line program *crs* is described here, including all input options.

## Running the COSMO-RS program

Running the COSMO-RS program involves the following steps:

- Construct an ASCII input file, say *in*.
- Run the program by typing (under UNIX):  
`$ADFBIN/crs <in >out`
- Move / copy relevant result files (in particular *CRSKF*) to the directory where you want to save them, and give them appropriate names.
- Inspect the standard output file *out* to verify that all has gone well.

## COSMO-RS and COSMO-SAC parameters

The COSMO-RS model has general parameters and element specific parameters. ADF's COSMO-SAC 2013-ADF model has general parameters, but also uses some of the COSMO-RS parameters, such as the element specific parameters. There are also technical and accuracy parameters, such as convergence criteria. This section explains how to set these parameters, and shows the default values for these parameters. By default the COSMO-RS method is chosen.

## COSMO-RS general parameters

```
CRSPARAMETERS
{RAV          rav}
{APRIME       aprime}
{FCORR        fcorr}
{CHB          chb}
{SIGMAHBOND   sigmahbond}
{AEFF         aeff}
{LAMBDA       lambda}
{OMEGA        omega}
{ETA          eta}
{CHORTF       chortf}
{combi1998 | combi2005}
{hb_all      | hb_hnof}
{hb_temp     | hb_notemp}
{fast        | nofast}
End
```

The ADF default values are optimized parameters for ADF calculations. The Klamt values can be found in Ref. [2]. See also Ref. [2] for the meaning of the parameters.

symbol	ADF Default Ref. [4]	ADF combi1998 Ref. [4]	Klamt Ref. [2]	MOPAC PM6
rav (rav)	0.400	0.415	0.5	0.400
aprime (a')	1510.0	1515.0	1288.0	1550.0
fcorr (fcorr)	2.802	2.812	2.4	2.802

chb (C <sub>hb</sub> )	8850.0	8850.0	7400.0	8400.0
sigmahbond (σ <sub>hb</sub> )	0.00854	0.00849	0.0082	0.00978
a <sub>eff</sub> (a <sub>eff</sub> )	6.94	7.62	7.1	5.96
lambda (λ)	0.130	0.129	0.14	0.135
omega (ω)	-0.212	-0.217	-0.21	-0.212
eta (η)	-9.65	-9.91	-9.15	-9.65
chortf (c <sup>⊥</sup> )	0.816	0.816	0.816	0.816
combi1998   combi2005	combi2005	combi1998	combi1998	combi2005
hb_all   hb_hnof	hb_hnof	hb_hnof	hb_hnof	hb_hnof
hb_temp   hb_notemp	hb_temp	hb_notemp	hb_notemp	hb_temp
fast   nofast	fast	fast	fast	fast

chortf

See Ref. [2] for the definitions:  $\sigma_v^\perp = \sigma_v^0 - c^\perp \sigma_v$

combi1998 | combi2005

If the subkey `combi1998` is included a thermodynamically inconsistent combinatorial contribution to the chemical potential  $\mu_i^{\text{comb}}$  of Ref.[2] is used. If the subkey `combi2005` is included (default) a thermodynamically consistent combinatorial contribution of Ref.[3] is used. See [the section on the combinatorial term](#) and Ref.[3].

hb\_all | hb\_hnof

If the subkey `hb_all` is included hydrogen bond interaction can be included between segments that belong to H atoms and all other segments. If the subkey `hb_hnof` is included (default) hydrogen bond interaction can be included only between segments that belong to H atoms that are bonded to N, O, or, F, and segments that belong to N, O, or F atoms.

hb\_temp | hb\_notemp

If the subkey `hb_notemp` is included the hydrogen bond interaction is not temperature dependent, as in Ref.[2]. If the subkey `hb_temp` is included (default) the hydrogen bond interaction is temperature dependent, as in Ref.[3]. See [the section on the temperature dependent hydrogen bond interaction](#) and Ref.[3].

fast | nofast

If the subkey `fast` is included the fast approximation is used. This fast approximation is the default. Use `nofast` for the original approach. See [the section on the fast approximation for COSMO-RS calculations](#).

## Links

COSMO-RS GUI tutorial: set COSMO-RS parameters [1]

## COSMO-RS element specific parameters

```
DISPERSION
{H dispH}
{C dispC}
{N dispN}
```

```
{...}  
End
```

The following table gives the element specific dispersion constants. The ADF default values are optimized parameters for ADF calculations. The Klamt values can again be found in Ref. [2]. The constants for F, Si, P, S, Br, and I in the ADF defaults were only fitted to a small number of experimental values or taken from Ref. [3].

element	ADF Default	ADF combi98	Klamt (Ref.[2])
H	-0.0340	-0.0346	-0.041
C	-0.0356	-0.0356	-0.037
N	-0.0224	-0.0225	-0.027
O	-0.0333	-0.0322	-0.042
Cl	-0.0485	-0.0487	-0.052
F	-0.026		
Si	-0.04		
P	-0.045		
S	-0.052		
Br	-0.055		
I	-0.062		

Note that not for all elements in the periodic system COSMO-RS parameters were fitted.

#### Links

COSMO-RS GUI tutorial: set COSMO-RS parameters [1]

## COSMO-SAC general parameters

The ADF COSMO-RS program can calculate activity coefficients using the COSMO-SAC 2013-ADF model, based on Ref. [9]. Like in the COSMO-RS method, pure compound vapor pressures can be given as input, for example, if experimental values are available. Note that if these values are not specified then the pure compound vapor pressure will be approximated using the COSMO-RS method, and not using the COSMO-SAC 2013-ADF method. Thus only the activity coefficients are calculated according to the COSMO-SAC 2013-ADF method. The COSMO-SAC 2013-ADF parameters in Ref. [9] are optimized parameters for use with ADF COSMO result files. Note that earlier COSMO-SAC methods [6,7] do not have parameters that were optimized for use with ADF COSMO result files. The key COSMOSAC2013 needs to be included if one wants to do a COSMO-SAC 2013-ADF calculation. For earlier COSMO-SAC methods one needs to include the key COSMOSAC.

```
COSMOSAC2013 | COSMOSAC  
SACPARAMETERS  
  {AEFF      aeff}  
  {FDECAY    fdecay}  
  {SIGMA0    sigma0}  
  {RN        rn}  
  {QN        qn}  
  {AES       aes}  
  {BES       bes}  
  {COHOH     cohoh}  
  {COTOT     cotot}  
  {COHOT     cohoh}  
  {OMEGA     omega}  
  {ETA       eta}  
  {RAV       rav}
```

```

    {QS      qs}
    {hb_temp | hb_notemp}
End

```

symbol	2013-ADF Xiong Ref. [9]	2010 Hsieh Ref. [7]	2007 Wang Ref. [6]
aeff (a <sub>eff</sub> )	6.4813	7.25	7.25
fdecay (f <sub>decay</sub> )	-	3.57	3.57
sigma0 (σ <sub>0</sub> )	0.01233	0.007	0.007
rn (r)	-	66.69	66.69
qn (q)	79.352	79.53	79.53
aes (AES)	7877.13	6525.69	8451.77
bes (BES)	0.0	1.4859 10 <sup>8</sup>	0.00
cohoH (COH-OH)	5786.72	4013.78	3484.42
cotoT (COT-OT)	2739.58	932.31	3484.42
cohoT (COH-OT)	4707.75	3016.43	3484.42
rav (r <sub>av</sub> )	0.51	-	-
qs (q <sub>s</sub> )	0.57	-	-
omega (ω)	-0.212	-0.212	-0.212
eta (η)	-8.00	-9.00	-9.00
hb_temp   hb_notemp	hb_notemp	hb_notemp	hb_notemp

See also Refs. [7,9] for the meaning of the parameters a<sub>eff</sub>, f<sub>decay</sub>, σ<sub>0</sub>, r, q, AES, BES, COH-OH, COT-OT, COH-OT, r<sub>av</sub>, q<sub>s</sub>. The parameter names in [6] have been translated into parameter names used in Ref. [7], by calculating AES from  $0.3 f_{\text{pol}} a_{\text{eff}}^{3/2} / (2\epsilon_0)$ , using BES = 0, and using COH-OH = COT-OT = COH-OT = c<sub>hb</sub>. The parameters f<sub>decay</sub> and r are not used in COSMO-SAC 2013-ADF [9]. The parameters r<sub>av</sub> and q<sub>s</sub> are not used in earlier COSMO-SAC methods [6,7]. The element specific COSMO-SAC 2013-ADF epsilon constants can be set with the block key EPSILON. These element specific epsilon constants can not be used in ADF's implementation of earlier COSMO-SAC methods.

The parameters ω, η and the element specific COSMO-RS dispersion constants are taken from the COSMO-RS model. They are not present in the COSMO-SAC 2013-ADF model (and earlier COSMO-SAC methods), but they are used in ADF's COSMO-SAC 2013-ADF implementation. Other COSMO-RS parameters are not used in ADF's COSMO-SAC 2013-ADF implementation, except the possibility to make the hydrogen bond parameter temperature dependent. The element specific COSMO-RS dispersion constants can be set with the block key DISPERSION. ω, η, and the element specific COSMO-RS dispersion constants are used in a COSMO-RS like method for the calculation of pure compound vapor pressures. This is different than the COSMO-SAC 2013-ADF method as described in Ref. [9]. The value of the COSMO-RS parameter η was reoptimized for ADF COSMO-SAC 2013-ADF calculations.

```
hb_temp | hb_notemp
```

If the subkey hb\_notemp is included (default) the hydrogen bond interaction is not temperature dependent, as in Refs. [6,7,9]. If the subkey hb\_temp is included the temperature dependence of the hydrogen bond interaction f<sub>hb</sub>(T) is the same as is described in [the section on the temperature dependent hydrogen bond interaction](#).

## COSMO-SAC element specific parameters

```

EPSILON
{H epsH}

```

```

| {C epsC}
| {N epsN}
| {...}
| End

```

The following table gives the element specific epsilon constants in case of COSMO-SAC 2013-ADF, see Ref. [9]. These element specific epsilon constants only have an effect in case of a mixture, in which case it will give a dispersion contribution to the calculated activity coefficients. Note that these only have an effect in the ADF's COSMO-SAC 2013-ADF implementation if one includes the COSMOSAC2013 key. Note also that these element specific epsilon constants in the ADF COSMO-SAC 2013-ADF implementation are not used for predicting vapor pressures of pure compounds. Like in the COSMO-RS method, pure compound vapor pressures can be given as input, for example, if experimental values are available. If these values are not specified then the pure compound vapor pressure will be approximated using the COSMO-RS method, and not using the COSMO-SAC 2013-ADF method. Thus only the activity coefficients are calculated according to the COSMO-SAC 2013-ADF method.

element	2013-ADF Xiong (Ref.[9])
H	338.13
C.sp3	29160.92
C.sp2	30951.83
C.sp	20685.98
N.sp3	23488.54
N.sp2	22663.34
N.sp	6390.40
O.sp3-H	8527.06
O.sp3	8484.38
O.sp2	6736.85
O.sp2-N	12145.28
Cl	8435.13
F	82512.21
P	56067.81
S	45065.19
Br	62947.83
I	105910.88

Note that not for all elements in the periodic system COSMO-SAC 2013-ADF parameters were fitted.

If one leaves the EPSILON block keyword empty the contribution of the mixture dispersion to the activity coefficient will be zero.

```

| EPSILON
| End

```

### Links

COSMO-RS GUI tutorial: Expert option: set COSMO-SAC 2013-ADF parameters [1]

## Technical and accuracy parameters

```

| TECHNICAL
| {RSCONV rsconv}
| {SACCONV sacconv}
| {MAXITER maxiter}
| {BPCONV bpconv}
| {BPMAXITER bpmaxiter}

```

```

{SOLCONV solconv}
{SOLMAXITER solmaxiter}
{SOLXILARGE solxilarge}
{EHDELTA ehdeltaT}
End

```

symbol	Default values
rsconv	$10^{-7}$ kcal/mol
sacconv	$10^{-7}$
maxiter	10000
bpconv	$10^{-6}$ bar
bpmaxiter	40
solconv	$10^{-5}$ molar fraction
solmaxiter	40
solxilarge	0.99 molar fraction
ehdeltaT	1.0 Kelvin

rsconv

Convergence criterion in kcal/mol in chemical potential calculation, not used in COSMO-SAC 2013-ADF. Default value  $1e-7$  kcal/mol.

sacconv

Convergence criterion in activity coefficient calculation, only used in COSMO-SAC 2013-ADF. Default value  $1e-7$ .

maxiter

Maximum number of cycles in chemical potential or activity coefficients calculation. Default value 10000.

bpconv

Convergence criterion (bar) for isobar or solvent boiling point calculation. Default value  $1e-6$  bar.

bpmaxiter

Maximum number of cycles in isobar or solvent boiling point calculation. Default value 40.

solconv

Convergence criterion (molar fraction) used in solubility calculations. Default value  $1e-5$  molar fraction.

solmaxiter

Maximum number of cycles in solubility calculation. Default value 40.

solxilarge

Threshold for (im-)miscibility (molar fraction) in solubility calculations. Above this value the mixture is considered to be fully miscible. Default value 0.99.

ehdeltaT

$\Delta T$  (Kelvin) used in the calculation of the excess enthalpy using the Gibbs-Helmholtz equation and in the calculation of the enthalpy of vaporization using the Clausius-Clapeyron equation using a numerical derivative with respect to  $T$ . Default value 1.0 Kelvin.

## Links

COSMO-RS GUI tutorial: set COSMO-RS or COSMO-SAC 2013-ADF parameters [1]

# Compounds

For each compound one has to add the keyword `COMPOUND`

```
COMPOUND filename
{cosmofile}
{drophbond}
{NRING nring}
{FRAC1 frac1}
{FRAC2 frac2}
{PVAP pvap}
{TVAP tvap}
{Antoine A B C}
{MELTINGPOINT meltingpoint}
{HFUSION hfusion}
{CPFUSION cpfusion}
{FLASHPOINT flashpoint}
{DENSITY density}
{SCALEAREA scalearea}
End
```

filename

The filename (can be a full path, otherwise relative path is assumed) should be a COSMO result file. How to make an ADF COSMO result file can be found [here](#).

cosmofile

If the subkey `cosmofile` is included the file should be an ASCII COSMO file (.cosmo). If not specified (default) the file should be a kf file, either an ADF COSMO result file TAPE21 (.t21) or a COSKF file (.coskf).

drophbond

If the subkey `drophbond` is included no hydrogen-bond terms will be included for this compound. If not specified (default) the hydrogen-bond terms are included for this compound.

nring

The number of ring atoms. This is a COSMO-RS parameter. It should be 6 for benzene, for example. Default value is 0.

frac1

The molar fraction of the compound in the solvent (mass fraction if the key `MASSFRACTION` is used). This is solvent 1 in case of the calculation of partition coefficients (Log P) or in case of a composition line.

frac2



The molar fraction of solvent 2 (mass fraction if the key `MASSFRACTION` is used), only used in case of the calculation of partition coefficients (Log P) or in case of a composition line.

`pvap, tvap`

Pure compound vapor pressure `pvap` (bar) at temperature `tvap` (Kelvin). Used only if both `pvap` and `tvap` are specified, and then will have an effect on the calculated vapor pressures or boiling points. Alternative is to set the Antoine coefficients. If both are not specified the pure compound vapor pressure is approximated using the COSMO-RS method.

`A, B, C`

A, B, and C are the pure compound Antoine coefficients, such that:

$$\log P = A - B/(T+C)$$

This Antoine equation is a 3-parameter fit to experimental pure compound vapor pressures P (bar) over a restricted temperature T (Kelvin) range. If the Antoine coefficients are specified this will have an effect on the calculated vapor pressures or boiling points. Alternative is to give input values for the pure compound vapor pressure at a fixed temperature. If both are not specified the pure compound vapor pressure is approximated using the COSMO-RS method.

`meltingpoint, hfusion, cpfusion`

Pure compound melting point `meltingpoint` (Kelvin), pure compound enthalpy of fusion `hfusion` (kcal/mol), and pure compound heat capacity of fusion `cpfusion` (kcal/(mol K)). Only used if both `meltingpoint` and `hfusion` are specified (`cpfusion` optional), and will then have an effect in solubility calculations if the temperature of the solvent is below the melting point.

`flashpoint`

Pure compound flash point `flashpoint` (Kelvin).

`density`

Pure compound density `density` (kg/L). Used for calculating the volume of a solvent molecule.

`scalearea`

Input scaling of COSMO surface area for a given compound. Default value 1.0 means the COSMO surface area is not scaled. Changing this value is an expert option, for example, to fit to experiment.

## Links

[COSMO-RS GUI tutorial: set pure compound parameters \[1\]](#)

## Temperature

```
| TEMPERATURE temperature {temperature_high ntemp}
```

`temperature`

Temperature (Kelvin) at which temperature the COSMO-RS calculation should take place. Default room temperature 298.15. The first temperature in case of a range of temperatures.

`temperature_high`

The last temperature (Kelvin) in case of a range of temperatures. Only used in case of solvent vapor pressure calculations or solubility calculations.

ntemp

The number of temperatures in case of a range of temperatures.

## Pressure

```
| PRESSURE pressure {pressure_high npress}
```

pressure

Pressure (bar) at which pressure the COSMO-RS calculation should take place. Default 1.01325 bar (1 atm). The first pressure in case of a range of pressures.

pressure\_high

The last pressure (bar) in case of a range of pressures. Only used in case of solvent boiling point calculations.

npress

The number of pressures in case of a range of pressures.

## Molar fractions and mass fraction

By default the ADF COSMO-RS program assumes molar fractions as input. This can be changed into mass fractions if one includes:

```
| MASSFRACTION
```

## Properties

### Vapor pressure

The vapor pressure of a mixture can be calculated with:

```
| PROPERTY vaporpressure  
End
```

In case of a mixture the mole fraction of each compound of the solvent should be given with the subkey `FRAC1` of the key `COMPOUND` for each compound. In case of a mixture also activity coefficients, and excess energies are calculated.

To calculate pure compound vapor pressures for more than one compound use:

```
| PROPERTY purevaporpressure  
End
```

It is possible to calculate the vapor pressure for a temperature range, see key `TEMPERATURE`.

The input pure compound vapor pressure will be used in the calculation of the vapor pressure of this compound if it is supplied with the key `COMPOUND` for this compound. If it is not specified then it will be approximated using the COSMO-RS method.

## Links

COSMO-RS GUI tutorial: solvent vapor pressure [1,2]

## Boiling point

The boiling point of a mixture can be calculated with the block key:

```
| PROPERTY boilingpoint  
| End
```

In case of a mixture the mole fraction of each compound of the solvent should be given with the subkey `FRAC1` of the key `COMPOUND` for each compound. In case of a mixture also activity coefficients, and excess energies are calculated.

To calculate pure compound boiling points for more than one compound use:

```
| PROPERTY pureboilingpoint  
| End
```

It is possible to calculate the boiling temperature for a pressure range, see key `PRESSURE`.

The input pure compound vapor pressure will be used in the calculation of the vapor pressure of this compound in the mixture if it is supplied with the key `COMPOUND` for this compound. If it is not specified then it will be approximated using the COSMO-RS method.

The COSMO-RS calculation of the boiling temperature of a solvent is performed with an iterative method. The temperature is varied until the calculated vapor pressure is within a certain threshold of the desired pressure.

## Links

COSMO-RS GUI tutorial: boiling point of a solvent [1]

## Solvent flash point

The flash point (lower flammable limit) of a compound is the lowest temperature at which the vapor of the compound forms an ignitable mixture in air. The COSMO-RS module can calculate the flash point of a mixture. The COSMO-RS module, however, does not calculate or predict the flash point of pure compounds. The COSMO-RS method is used to calculate the partial vapor pressures of each compound in the mixture, and it uses Le Chatelier's mixing rule to calculate the flash point of this mixture in the gas phase. Input pure compound flash points should be provided by the user, with the subkey `FLASHPOINT` `flashpoint` of the key `COMPOUND`.

```
| PROPERTY flashpoint  
| End
```

The mole fraction of each compound of the solvent should be given with the subkey `FRAC1` of the key `COMPOUND` for each compound.

## Partition coefficients (LogP)

The partition coefficient of a compound in a mixture of two immiscible solvents, can be calculated with:

```
PROPERTY logp
{VOLUMEQUOTIENT volumequotient}
End
```

volumequotient

If the subkey `VOLUMEQUOTIENT` is included the `volumequotient` will be used for quotient of the molar volumes of solvent 1 and solvent 2 instead of calculated values.

The mole fraction of each compound of the solvent 1 and solvent 2 should be given with the subkey `FRAC1` and subkey `FRAC2` of the key `COMPOUND` for each compound, respectively. In case of partly miscible liquids, like, for example, the Octanol-rich phase of Octanol and Water, both components have nonzero mole fractions. The compounds that are included without a given mole fraction are considered to be infinite diluted solutes. The partition coefficients are calculated for all compounds.

One can use some compounds that are present in `ADFHOME/atomicdata/ADFCRS` (Water, 1-Octanol, Benzene, Ethoxyethane, Hexane), or one can use compounds from the `ADFCRS-2010` database. For example, for Octanol/Water partition coefficients one can use:

```
Property logp
  VolumeQuotient 4.93
End
Compound "$ADFHOME/atomicdata/ADFCRS/1-Octanol.coskf"
  frac1 0.725
End
Compound "$ADFHOME/atomicdata/ADFCRS/Water.coskf"
  frac1 0.275
  frac2 1.0
End
```

## Links

COSMO-RS GUI tutorial: partition coefficients (log P) [1,2], Octanol-Water partition coefficients (log Pow) [1]

## Activity coefficients solvent and solute

The mole fraction of each compound of the solvent should be given with the subkey `FRAC1` of the key `COMPOUND` for each compound. The compounds that are included without a given mole fraction are considered to be infinite diluted solutes. The activity coefficients are calculated for all compounds.

```
PROPERTY activitycoef
{DENSITYSOLVENT densitysolvent}
End
```

densitysolvent

If the subkey `DENSITYSOLVENT` is included the `densitysolvent` will be used for the density of the solvent (kg/L) instead of calculated values. Relevant for the calculation of the Henry's law constant.

The input pure compound vapor pressure will be used in the calculation of the partial vapor pressure of this compound in the mixture if it is supplied with the key `COMPOUND` for this compound. If it is not specified then it will be approximated using the COSMO-RS method. Relevant for the calculation of the Henry's law constant.

The Henry's law constants are calculated in 2 units. The Henry's law constant  $k_H$  is the ratio between the liquid phase concentration of a compound and its partial vapor pressure in the gas phase. The

dimensionless Henry's law constant  $k_H^{CC}$  is the ratio between the liquid phase concentration of a compound and its gas phase concentration.

Also calculated is  $\Delta G_{\text{solV}}^{\text{liq-solv}}$ , which is the solvation Gibbs free energy from the pure compound liquid phase to the solvated phase, and  $\Delta G_{\text{solV}}^{\text{gas-solv}}$ , which is the solvation Gibbs free energy from the pure compound gas phase to the solvated phase, with a reference state of 1 mol/L in both phases. In addition a Gibbs free energy is calculated which is the free energy of the solvated compound with respect to the gas phase energy of the spin restricted spherical averaged neutral atoms, the compound consist of. Note that zero-point vibrational energies are not taken into account in the calculation of this free energy. This energy could be used in the calculation of  $pK_a$  values.

### Links

COSMO-RS GUI tutorial: activity coefficients [1,2], solvation free energies [1], Henry's law constants [1],  $pK_a$  values [1]

## Solubility

The solubility of solutes in 1 mixture can be calculated with:

```
| PROPERTY solubility  
| End
```

The mole fraction of each compound of the solvent should be given with the subkey `FRAC1` of the key `COMPOUND` for each compound, and should add up to 1.0. The solutes should have zero molar fraction in the solvent.

The solubility of 1 solute in pure solvents can be calculated with

```
| PROPERTY puresolubility  
| End
```

The mole fraction of each pure solvent should be 1.0, and should be set the subkey `FRAC1` of the key `COMPOUND` for each compound. The solute should have zero molar fraction in the solvent.

It is possible to calculate the solubility of a solute at a temperature range, see key `TEMPERATURE`.

For solubility calculations of a solid compound one should add the pure compound melting point  $T_m$ , pure compound enthalpy of fusion  $\Delta H_{\text{fus}}$ , and optionally the pure compound heat capacity of fusion  $\Delta C_p$  using the subkeys `meltingpoint`, `hfusion`, and `cpfusion`, respectively, of the key `COMPOUND` for this compound. The COSMO-RS method does not predict these  $\Delta H_{\text{fus}}$ ,  $\Delta C_p$ , or  $T_m$ .

The assumption made in the solubility calculation may be invalid in case of a solubility of a liquid in a solvent, especially if the solubility of the solvent in the liquid is high. For binary systems one may check this by calculating the miscibility gap in the binary mixture of the two liquids.

It is possible to calculate the solubility of a gas in a solvent, if one adds the subkey `isobar` and adds the partial vapor pressure `partialvaporpressure` (bar) of the gas as argument for the key `PRESSURE`:

```
| PROPERTY solubility  
|   isobar  
| End  
| PRESSURE partialvaporpressure
```

The solubility of a gas in a solvent can also be calculated using Henry's law, which is valid for ideal dilute solutions, see see the key `PROPERTY activitycoef`.

The COSMO-RS calculation of the solubility of a compound is performed with an iterative method, since the activity coefficient of the compound depends on the molar fraction of this compound.

#### Links

COSMO-RS GUI tutorial: solubility [1,2]

## Binary mixture (VLE/LLE)

The COSMO-RS module can automatically calculate properties of a binary mixture, by calculating these properties for a number of different compositions.

Exactly two compounds should be given in the input file.

```
PROPERTY binmixcoef
{Nfrac nfrac}
{isotherm | isobar | flashpoint}
End
```

`nfrac`

Number of different mixtures for which the binary mixture is calculated will be `nfrac+5`. Default value for `nfrac` is 10, which means 15 different mixtures.

`isotherm | isobar | flashpoint`

If the subkey `isotherm` is included (default) the binary mixture will be calculated at a fixed temperature. If the subkey `isobar` is included the binary mixture will be calculated at a fixed vapor pressure. If the subkey `flashpoint` is included the flash point of the binary mixture will be calculated.

The input pure compound vapor pressure will be used in the calculation of the partial vapor pressure of this compound in the mixture if it is supplied with the key `COMPOUND` for this compound. If it is not specified then it will be approximated using the COSMO-RS method.

In case of a miscibility gap (LLE) data of the 2 immiscible liquid phases will be calculated. Also information about possible azeotropes will be calculated. With the COSMO-RS GUI, activity coefficients, (partial) vapor pressures, and excess energies can be viewed.

#### Links

COSMO-RS GUI tutorial: vapor-liquid diagram binary mixture (VLE/LLE) [1,2]

## Ternary mixture (VLE/LLE)

The COSMO-RS module can automatically calculate properties of a ternary mixture, by calculating these properties for a number of different compositions.

Exactly three compounds should be given in the input file.

```
PROPERTY ternarymix
{Nfrac nfrac}
{isotherm | isobar | flashpoint}
End
```

nfrac

Number of different mixtures for which the ternary mixture is calculated will be  $(nfrac+1)*(nfrac+2)/2$ . Default value for nfrac is 10, which means 55 different mixtures.

isotherm | isobar | flashpoint

If the subkey `isotherm` is included (default) the ternary mixture will be calculated at a fixed temperature. If the subkey `isobar` is included the ternary mixture will be calculated at a fixed vapor pressure. If the subkey `flashpoint` is included the flash point of the ternary mixture will be calculated.

The input pure compound vapor pressure will be used in the calculation of the partial vapor pressure of this compound in the mixture if it is supplied with the key `COMPOUND` for this compound. If it is not specified then it will be approximated using the COSMO-RS method.

In case of a miscibility gap liquid-liquid equilibrium (LLE) data such as tie lines and an approximate phase diagram, are calculated. With the COSMO-RS GUI, activity coefficients, (partial) vapor pressures, and excess energies can be viewed as a colormap in a 2-dimensional plot with 2 of the liquid compositions on the axes.

## Solvents s1 - s2 Composition Line

The COSMO-RS module can linear interpolate between the compositions of solvent 1 and solvent 2, which both could be mixtures, and calculate properties, like activity coefficients, and excess energies. This property calculation does not calculate a possible miscibility gap.

The mole fraction of each compound of the solvent 1 and solvent 2 should be given with the subkey `FRAC1` and subkey `FRAC2` of the key `COMPOUND` for each compound, respectively.

```
| PROPERTY compositionline  
| {Nfrac nfrac}  
| {isotherm | isobar | flashpoint}  
| End
```

nfrac

Number of different mixtures of the 2 solvents is calculated will be  $(nfrac+1)$ . Default value for nfrac is 10, which means 11 different mixtures.

isotherm | isobar | flashpoint

If the subkey `isotherm` is included (default) a fixed temperature will be used. If the subkey `isobar` is included a fixed vapor pressure will be used. If the subkey `flashpoint` is included the flashpoint will be calculated.

## Analysis

### Sigma profile

The sigma profile of a mixture can be calculated with:

```
| PROPERTY sigmaprofile  
| {Nprofile nprofile}
```

```
{SigmaMax sigmamax}  
End
```

In case of a mixture the mole fraction of each compound in the mixture should be given with the subkey `FRAC1` of the key `COMPOUND` for this compound.

The sigma profile pure compounds can be calculated with:

```
PROPERTY puresigmaprofile  
{Nprofile nprofile}  
{SigmaMax sigmamax}  
End
```

nprofile

Number of data points for which to calculate the sigma profile. default value 50.

sigmamax

The sigma profile is calculated between `-sigmamax` and `sigmamax`. Default value 0.025.

The hydrogen bonding part (HB) of the sigma profile(s) will also be calculated. In case of a COSMO-SAC 2013-ADF calculation also the OH component of hydrogen bonding (HB-OH) is calculated, and the other type component of hydrogen bonding (HB-OT) is calculated.

#### Links

COSMO-RS GUI tutorial: sigma profile [1]

## Sigma potential

The sigma potential of a mixture can be calculated with:

```
PROPERTY sigmapotential  
{Nprofile nprofile}  
{SigmaMax sigmamax}  
End
```

In case of a mixture the mole fraction of each compound in the mixture should be given with the subkey `FRAC1` of the key `COMPOUND` for this compound.

The sigma profile pure compounds can be calculated with:

```
PROPERTY puresigmapotential  
{Nprofile nprofile}  
{SigmaMax sigmamax}  
End
```

nprofile

Number of data points for which to calculate the sigma potential. default value 50.

sigmamax

The sigma potential is calculated between `-sigmamax` and `sigmamax`. Default value 0.025.

#### Links

COSMO-RS GUI tutorial: sigma potential [1]



## COSMO-RS command line utilities

The two COSMO-RS command line utility programs *kf2cosmo* and *cosmo2kf* convert COSMO kf files from binary to ASCII and vice versa.

```
| kf2cosmo file.coskf file.cosmo
```

*kf2cosmo* reads from the kf file *file.coskf* (should exist) the section 'COSMO' and writes to the ASCII file *file.cosmo* (should not exist). Instead of a *.coskf* file, the file can also be a TAPE21 file which is a result file from an ADF COSMO calculation.

```
| cosmo2kf file.cosmo file.coskf
```

*cosmo2kf* reads from the ASCII file *file.cosmo* (should exist) and writes a section 'COSMO' to the kf file *file.coskf* (should not exist). Note that only a section 'COSMO' is written to the kf file, which means that this file can not be used like an ordinary TAPE21 (.t21) file.

```
| cosmo2kf file.cos file.coskf
```

*cosmo2kf* can also read a MOPAC COSMO result file *file.cos* (should exist and should have the file extension *.cos*) and writes a section 'COSMO' to the kf file *file.coskf* (should not exist).

```
| cpkf file.t21 file.coskf COSMO
```

With the ADF kf utility *cpkf* one can copy the section 'COSMO' from a *file.t21* (should exist) to a *file.coskf* (should not exist). The file *file.t21* should be a result of an ADF COSMO calculation. The file *file.coskf* is much smaller than *file.t21*. This file *file.coskf* can not be used like an ordinary *.t21* file, but it contains all necessary information such that it can be used as input for a COSMO-RS calculations.

With the ADF kf utilities *dmpkf* and *udmpkf* one can also convert COSMO kf files from binary to ASCII and vice versa.

```
| dmpkf file.coskf > ascii_result  
| udmpkf < ascii_result newfile.coskf
```

## References

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