

Our products:

- **COSMOtherm**

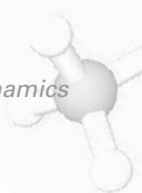
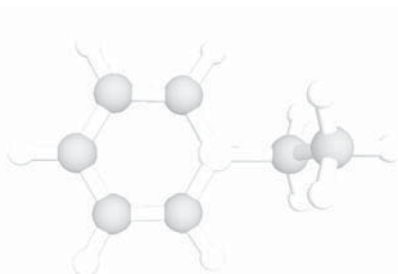
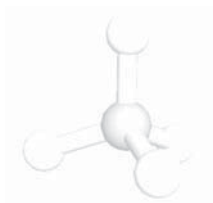
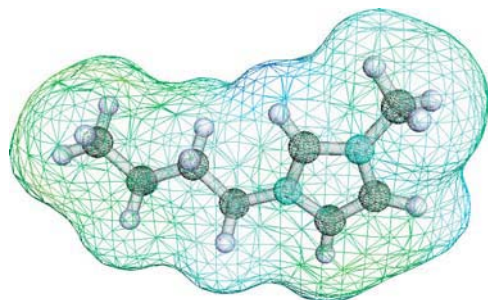
A fast implementation of the COSMO-RS theory for the prediction of thermodynamic properties of solutions.

- **COSMObasell**

A collection of COSMO files of ions of common ILs.

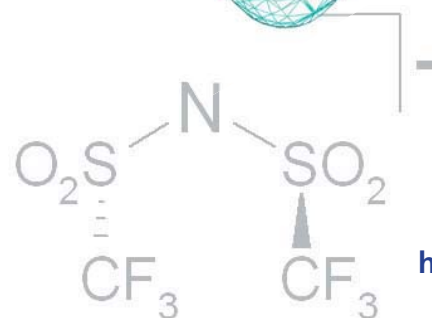
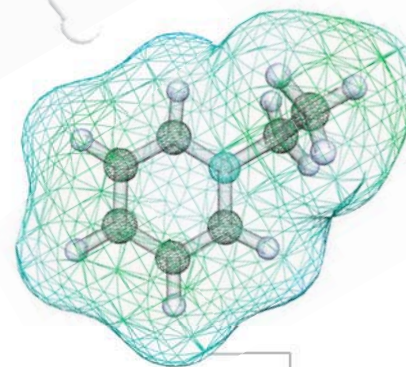
- **Consulting**

We offer research and consulting service in the field of thermodynamic property prediction of solutions.



COSMOtherm & COSMObasell

Property prediction of Ionic Liquid mixtures



COSMOlogic

GmbH & Co. KG

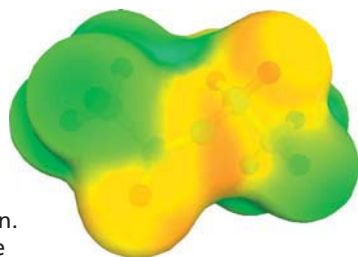
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Computational Chemistry and Fluid Thermodynamics

Burscheider Str. 515
D-51381 Leverkusen
Tel.: 49 (0) 2171 73168 0
Fax: 49 (0) 2171 73168 9
E-mail: info@cosmologic.de
Web: <http://www.cosmologic.de>
CEO: Dr. Andreas Klamt

<http://www.cosmologic.de>

COSMOtherm for Ionic Liquids

Their environmental and economic benefits have led to the rapid development and application of ionic liquids in process chemistry. The ever-growing set of cations and anions for ionic liquids increases the challenge of finding the best combination or mixture for a given application. COSMOtherm provides very easy, fast and accurate prediction of properties of solutes in ionic liquids and their mixtures. The quantum chemical basis of the method allows it to be used in the design of new tailor-made ionic liquids, by predicting properties of unknown, hypothetical anions and cations and their mixtures.



NH₃ / IL mixtures

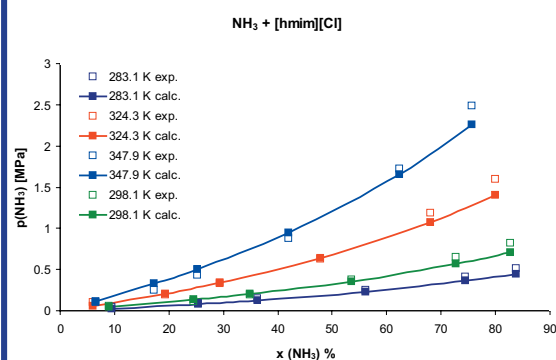


Fig. 2. VLE of a NH₃ / [hmim][Cl] mixture. Exp. data from ref. 2.

COSMObaseIL the Ionic Liquid (IL) database

COSMObaseIL is a database of 71 cations and 32 anions of COSMO-files of the most common ILs. These files can be used for the calculation of properties of solutes in IL mixtures. The database includes all the information needed by COSMOtherm. The graphical user interface (GUI) of COSMOtherm makes it fast and easy to use.

ln(γ^{inf}) Predictions

ln(γ^{inf}) Deviations from Exp. Data³ (all Temp. and Solutes)

IL	RMS	Data Points	Max. Deviation
[bmim][N(SO ₂ CF ₃) ₂]	0.29	52	0.60 (heptane, 20°C)
[emim][N(SO ₂ CF ₃) ₂]	0.31	80	0.78 (heptane, 20°C)
[N-ethylpyridinium][N(SO ₂ CF ₃) ₂]	0.40	122	1.02 (octane, 30°C)
[mmim][N(SO ₂ CF ₃) ₂]	0.51	54	1.11 (heptane, 30°C)
[pyridinium][C ₂ H ₅ OC ₂ H ₄ OSO ₃]	0.91	56	1.42 (1-pentene, 50°C)
[ocmim][Cl]	0.93	45	1.30 (pentane, 25°C)
[emim][C ₂ H ₅ OSO ₃]	1.21	42	1.74 (heptane, 30°C)
[mmim][CH ₃ OC ₂ H ₄ OSO ₃]	1.51	56	2.26 (1-heptene, 40°C)
[mmim][CH ₃ OSO ₃]	1.55	56	2.34 (1-heptene, 30°C)
[mmim][(CH ₃ O) ₂ PO ₂]	1.66	59	2.96 (1-octene, 30°C)

Fig. 3. Activity coefficients at infinite dilution of various solutes in 10 ILs.

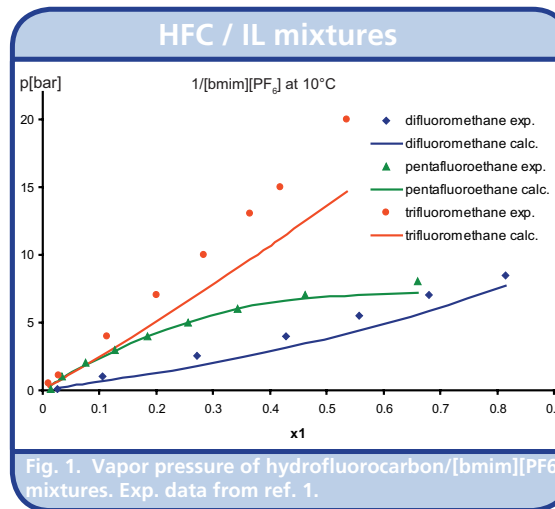


Fig. 1. Vapor pressure of hydrofluorocarbon/[bmim][PF₆] mixtures. Exp. data from ref. 1.

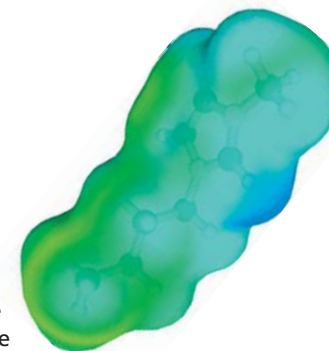
Applying COSMOtherm to IL solutions

The key value calculated in a COSMOtherm run is the chemical potential of the compounds in solution. Using this data the program can calculate a wide range of thermodynamic equilibrium properties. Although the treatment of ILs is slightly different than for normal solvents properties of solutes in IL solutions are easily accessible, e.g.:

- Activity Coefficients of solutes in IL solutions
- VLEs of IL containing mixtures
- LLEs of IL/solvent mixtures
- Partitioning coefficients between IL and other phases

IL screening

The fast and easy calculation of activity coefficients or partitioning coefficients with COSMOtherm allows for a fast solubility screening of solutes in ILs or the partitioning between two arbitrary phases including ILs.



References

- 1) M. B. Shiflett, A. Yokozeki, *AIChE Journal* 52 (2005), 1205.
- 2) A. Yokozeki, M. B. Shiflett, *Ind. Eng. Chem. Res.* 46 (2007), 1605-1610.
- 3) R.Kato, J. Gmehling, *Fluid Phase Equilibria* 226 (2004), 37-44. M. Krummen, P. Wasserscheid, J. Gmehling, *J. Chem. Eng. Data* 47 (2002), 1411-1417. W. David, T. M. Letcher, D. Ramjugernath J. D. Raal, *J. Chem. Thermodynamics* 35(2003), 1335-1341.
- 4) A. Heintz, J. K. Lehmann, C. Wertz, *J. Chem. Eng. Data* 48(3) (2003), 472-474.

LLE Predictions

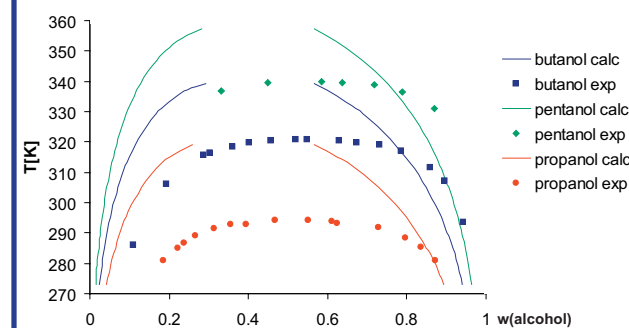


Fig. 4. LLE predictions of alcohols in [emim][NTf₂]. Exp. data from ref. 4.