37l Teaching Molecular Thermodynamics with Cosmotherm

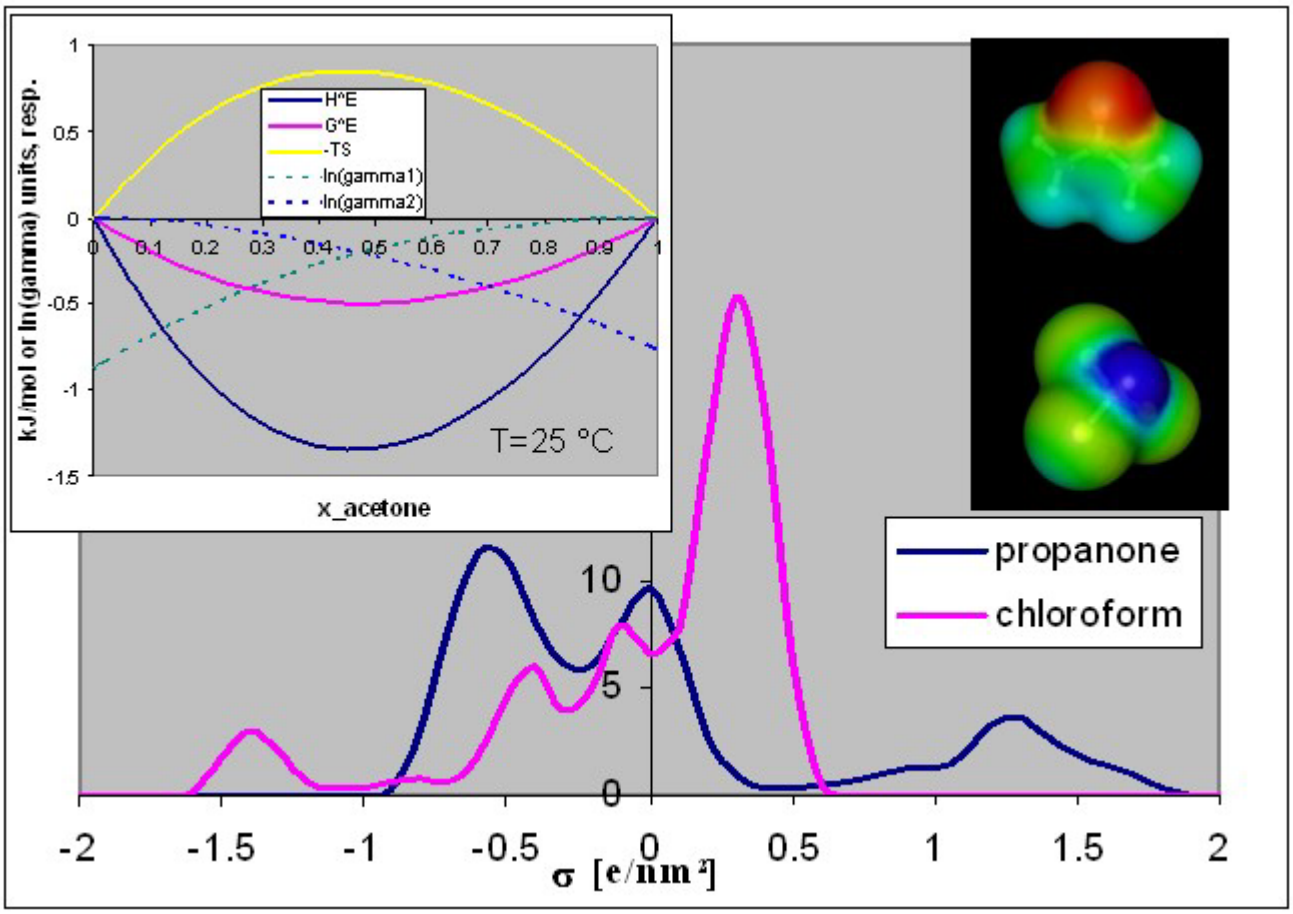
Andreas Klamt

Our COSMO-RS method for the calculation of molecular fluid phase thermodynamics based on quantum chemical calculations has become widely accepted as a very fundamental, vivid, and powerful method for thermodynamic calculations in liquids. Beyond its high predictive power for demanding molecules, its concept of surface interactions quantified by the quantum chemically derived surface polarization charges σ provides a very graphical insight into the interactions of molecules and to the relation of these interactions with the thermodynamics of pure and mixed liquid systems. In contrast to most other methods, COSMO-RS can visualize and explain the entire pathway from molecules to mixture phase diagrams, without introducing abstract and dry entities as interaction parameters. In this way it can be used in a unique way to teach why some molecules like each other and others do not, why some very different molecules may behave as ideal mixtures and other similar molecules show very non-ideal behaviour, and many other interesting questions.

With our graphical user interface COSMOthermX we have packaged an educational version COSMOthermEDU, which comes with a variety of quantum chemically pre-calculated COSMO files for common compounds and solvents. This allows you to demonstrate interactively how chemistry and interactions of molecules are related to thermodynamics. You can visualize molecular surface polarities, compare σ-profiles, calculate and compare σ-potentials, and generate binary phase diagrams interactively.

You can hand the program out to your students and let them study and discuss the differences of some molecules and how these differences cause different phase behaviour, which effect temperature has on some phase diagrams, why some are more sensitive to temperature than others, …

Thus COSMOthermEDU can turn the dry subject of thermodynamics into a vivid and colourful experience for the students which they at least will keep in their minds for long.


H^E
G^E
-TS
ln(gamma1)
ln(gamma2)
T=25 °C
kJ/mol or ln(gamma) units, resp.
x_acetone
propanone
chloroform
σ [e/nm²]