# CPP 32: Poster: Liquids and Ionic Liquids

Time: Wednesday 17:30–19:00 Location: Poster C

CPP 32.1 Wed 17:30 Poster C

**Additivity of the heats of transport in binary liquids** —
•Steffen Hartmann[1], Gerhard Wittko[1], Werner Köhler[1],
Katja Albers[2], Feely Rüther[2], and Gabriele Sadowski[2] —
[1]Physikalisches Institut, Universität Bayreuth — [2]Fakultät Bio- und
Chemieingenieurwesen, Universität Dortmund

The coupling between heat and mass transport in multicomponent
systems under the presence of a temperature gradient is quantitatively
expressed by the Soret coefficient. This coefficient contains true non-
equilibrium quantities, the so-called heats of transport, and a thermo-
dynamic factor that can be obtained from equilibrium properties. We
have measured the Soret coefficients of a large number of binary mix-
tures of organic solvents and found an additive model for the heats of
transport of equimolar mixtures with a high correlation between pre-
dicted and measured values. The necessary thermodynamic factors,
which contain the activity coefficients, have been determined from the
PC-SAFT equation of state and the group contribution method Modi-
fied UNIFAC (Dortmund). Our results show, how the components can
be ordered according to their thermophobicity.

CPP 32.2 Wed 17:30 Poster C

**Measurement of diffusion and thermal diffusion in ternary
mixtures.** — •Andreas Königer and Werner Köhler —
Physikalisches Institut, Universität Bayreuth

The molecular diffusion process in ternary mixtures is much more com-
plicated than that in binaries, because of additional cross diffusion
coefficients.

We have developed a highly sensitive two-color beam deflection tech-
nique to measure diffusion and thermal diffusion in ternary fluid mix-
tures. Simultaneous detection of two laser beams with different wave-
lengths makes it possible to determine the concentration profile of all
three components. By comparing the measured beam deflection signal
to a numerical solution of the coupled heat and mass transport equa-
tions, the diffusion matrix and the thermal diffusion coefficients can
be obtained by a non-linear least squares fitting routine.

We report on first measurements of the Soret-, thermal diffusion,
and diffusion coefficients, including cross diffusion, of a mixture con-
sisting of tetralin, dodecane and isobutylbenzene, which are known as
reference systems for thermal diffusion in binary mixtures.

CPP 32.3 Wed 17:30 Poster C

**Temperature dependent structure of liquid water investi-
gated by means of energy-dispersive X-ray diffraction and
molecular dynamic simulations** — •Christa Guse, Arnold
Simionescu, Benjamin Schünemann, Reinhard Hentschke, and
Hartwin Bomsdorf — Fachbereich Mathematik und Naturwis-
senschaften, Bergische Universität, D-42097 Wuppertal, Germany

X-ray diffraction is investigated in the supercooled region (-10° C to 0°
C) and, for comparison, at ambient conditions. By means of an energy-
dispersive setup coherent X-ray scatter cross-sections within a wide
range of momentum transfer values are monitored simultaneously us-
ing relatively simple laboratory equipment. The data are corrected for
the energy dependent detector response, geometric broadening effects,
sample absorption and Compton-scattering. The corrected diffraction
curves are in good agreement with results from the ALS experiment.
Additional comparisons with available literature data and with com-
puter simulation results of different rigid water models are presented,
relating the scattering intensities to the microscopic H-bond structure
and dynamics.

CPP 32.4 Wed 17:30 Poster C

**Tracking vapor-liquid coexistence in fluids of charged soft
dumbbells** — •Heiko Braun and Reinhard Hentschke — Fach-
bereich Mathematik und Naturwissenschaften
Bergische Universität, D-42097 Wuppertal, Germany

The existence of gas-liquid coexistence in dipolar fluids with no other
contribution to attractive interaction than dipole-dipole interaction is
a basic and open question in the theory of fluids. Recent Monte Carlo
work by Camp and co-workers indicates that a fluid of charged hard
dumbbells does exhibit gas-liquid (g-l) coexistence. This system has
the potential to answer the above fundamental question because the
charge-to-charge separation, $d$, on the dumbbells may be reduced to,
at least in principle, yield the dipolar fluid limit. Using the molecular-
dynamics technique we present simulation results for the g-l critical
point of charged soft dumbbells at fixed dipole moment as function of
$d$. We do find a g-l critical point at finite temperature even at the
smallest $d$ value ($10^{-4}$). Reversible aggregation appears to play less a
role than in related model systems as $d$ becomes small. Consequently
attempts to interpret the simulation results using either an extension
of Flory's lattice theory for polymer systems, which includes reversible
assembly of monomers into chains, or the defect model for reversible
networks proposed by Tlusty and Safran are not successful. The over-
all best qualitative interpretation of the critical parameters is obtained
by considering the dumbbells as dipoles immersed in a continuum di-
electric.

CPP 32.5 Wed 17:30 Poster C

**Dipolar particles in an external field: Molecular dynamics
simulation and mean field theory** — •Ran Jia and Reinhard
Hentschke — Fachbereich Mathematik und Naturwissenschaften,
Bergische Universität, D-42097 Wuppertal, Germany

Using Molecular Dynamics computer simulation we compute gas–
liquid phase coexistence curves for the Stockmayer fluid in an external
electric field. We observe a field induced shift of the critical tempera-
ture, $\Delta T_c$. The sign of $\Delta T_c$ depends on whether the potential or the
surface charge density is held constant, assuming that the dielectric
material fills the space between capacitor plates. Our own as well as
previous literature data for $\Delta T_c$ are compared to and interpreted in
terms of a simple mean field theory. Despite considerable errors in the
simulation results, we find consistency between the simulation results
obtained by different groups including our own and the mean field de-
scription. The latter ties the sign of $\Delta T_c$ to the outside constraints via
the electric field dependence of the orientation part of the mean field
free energy.