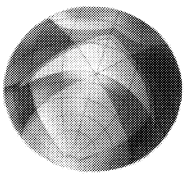
Deutsche Bunsen-Gesellschaft für Physikalische Chemie

76th International Bunsen Discussion Meeting
Global Phase Diagrams

August 19-22, 2001
Conference Center Walberberg, Germany

Book of Abstracts



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Thomas Kraska (Editor)

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The 76th International Bunsen Discussion Meeting *Global Phase Diagrams*

The German Bunsen Society of Physical Chemistry supports different kinds of meetings and conferences. Besides the annual meeting, which is held each year in May or early June, the Bunsen Colloquium and the International Bunsen Discussion Meetings are endorsed. The Bunsen Colloquium are usually small one-day meetings about a certain topic. The International Bunsen Discussion Meetings are held two or three times a year each on a current topic in the area of physical chemistry. In the area of global phase diagrams a Bunsen-Colloquium has been held in March 1999. Papers presented at this meeting have been published in PCCP **1**, 4225-4336 (1999) and **2**, 91-95 (2000). The focus of this international discussion meeting is on topical developments in the area of phase diagrams and their modelling based on molecular interactions. This effort is an important basis for the investigation of the properties of matter as well as a basis for the development of innovative processes.

About the Venue of the Conference

Walberberg is a small village with 4000 inhabitants which has already been a settlement 500 years A.D.. From the street map one can still recognize the structure of a Roman street village. The name “Walburgisberg” or “Walberberg” goes back to time when the bishop of Cologne in 1070 sent the relics of the saint Walburgis to Walberberg for protection. In the 12th Century the Cistercians founded an abbey next to the parish church. In 1447 the Cistercians of Heisterbach took over, followed by the Jesuits in 1591. The Later the Jesuits converted the an old water castle on the slope above the village to a convent which is now the Dominican convent St. Albert where the conference takes place.

The 12th and 13th Century were characterized by an increasing enstrangement of the people and the church, which led to superstition, formation of sects, and political unrest. Dominicus felt the need of the people of his time and in 1217 founded the order of the preachers (ordo praedicatorum=Dominicans). He understood that the church needed a community of educated preachers who faced the problems of the time and were able to provide competent spiritual guidance. When Dominicus died in 1221 the new order was already prospering. Even before his death he sent the first Dominicans to Cologne to build up the order in this region. The Dominican cloister in Cologne became its spritual center. Moreover, Cologne became a focus of science at this time because of Albert of Lauingen, who was admitted to the order by a successor of Dominicus. Albert of Lauingen, later called Albertus Magnus, is considered a founding father of the University at Cologne. One of his students was Thomas of Aquin, well known as probably the most famous and most influential theologian of the Middle Ages.

The Dominicans founded their convent in Walberberg in 1926. It took up studies in 1934. After World War II a christian social educational center for adults was added to it. Since that time more and more people came to Walberberg for seminars or congresses. A new wing of the building was built with a library and seminar rooms. The library is one of the major theological libraries of Germany. It is especially famous for its collection of rare old books (incunabula).

Time table

Sunday, August 19

14.00 – 18.00	*Registration*
18.00 – 19.00	*Dinner*
20.00 – 21.00	Prausnitz (p 17)

Monday, August 20

08.45 – 09.30	de Loos (p 21)
09.30 – 10.00	Thiéry (p 22)
10.00 – 10.30	Segura (p 23)
10.30 – 11.00	*Coffee Break*
11.00 – 11.45	Valyashko (p 24)
11.45 – 12.05	Bumba (p 26)
12.05 – 12.25	Groß (p 27)
12.30 – 14.00	*Lunch*
14.00 – 14.45	Findenegg (p 28)
14.45 – 15.05	Brovchenko (p 29)
15.05 – 15.25	Imre (p 30)
15.25 – 15.45	Anisimov (p 31)
15.45 – 16.15	*Coffee Break*
16.15 – 16.45	Schneider (p 32)
16.45 – 17.15	Peters (p 33)
17.15 – 17.35	Nieuwoudt (p 34)
17.35 – 17.55	Scheidgen (p 35)
18.00 – 19.00	*Dinner*
20.00 – 22.00	Poster Session

Tuesday, August 21

08.45 – 09.30	Maurer (p 39)
09.30 – 09.50	Salminen (p 40)
09.50 – 10.10	Toikka (p 41)
10.10 – 10.30	Blagov (p 43)
10.30 – 11.00	*Coffee Break*
11.00 – 11.45	Vega (p 44)
11.45 – 12.05	Francesconi (p 45)
12.05 – 12.25	Valentin (p 46)
12.30 – 14.00	*Lunch*
14.00 – 14.45	Kofke (p 47)
14.45 – 15.15	Kvamme (p 48)
15.15 – 15.45	Kohli (p 49)
15.45 – 16.15	*Coffee Break*
16.15 – 16.35	Boublík (p 50)
16.45 – 17.15	Filipe (p 51)
17.15 – 17.45	Sadus (p 52)
18.00 – 19.00	*Dinner*
20.00 – 21.00	*Concert*

Wednesday, August 22

08.45 – 09.30	Brennecke (p 55)
09.30 – 09.50	Dąbrowska (p 56)
09.50 – 10.10	Galicia-Luna(p 57)
10.10 – 10.30	Goodarzina (p 58)
10.30 – 10.50	*Coffee Break*
10.50 – 11.10	Oleinikova (p 59)
11.10 – 11.30	Lopes (p 61)
11.30 – 11.50	Polishuk (p 62)
12.15 – 14.00	*Lunch*

Scientific Programme

Oral Presentations

Sunday, August 19, 20.00-21.00
J. M. Prausnitz (*invited*)
A thermodynamic frontier: phase diagrams for modern chemical technology

Monday, August 20
Mornig I, 8.45-10.30
T. W. de Loos (*invited*)
The interference of fluid phase equilibria and solid-fluid equilibria

R. Thiéry, S.N. Lvov, J. Dubessy
A global phase diagram for the ion-dipole model in the mean spherical approximation

G. Fernández, H. Segura, T. Kraska, I. Polishuk, J. Wisniak
On the global phase diagram for Lennard-Jones mixtures

Morning II, 11.00-12.25
V. M. Valyashko (*invited*)
Complete phase diagrams of ternary systems with one volatile component and immiscibility in two of the constituent binary mixtures.

J. Bumba, J. Kolafa, A. Malijevský, J. Veverka
Global phase diagram of augmented van der Waals equation of state. Entropy driven phase separation for mixtures of hard spheres.

D. H. E. Groß
Phase transitions and second law without thermodynamic limit

Afternoon I, 14.00-15.45
G. H. Findenegg, S. Groß, Th. Michalski, A. Schreiber, M. Thommes (*invited*)
Pore condensation, hysteresis and criticality of fluids in materials with uniform pores and disordered pore systems

I. Brovchenko, A. Geiger, A. Oleinikova
Liquid-vapour phase diagrams of water in nanopores: confinement vs surface effects

A. R. Imre, T. Kraska, B. A. Wolf, L. V. Yelash
The effect of pressure on the liquid-liquid phase equilibrium of a blend of two polydisperse polyalkylsiloxanes

M. A. Anisimov
Novel phase transition behavior in isotropic fluids: beyond liquid-liquid demixing

Afternoon II, 16.15-17.55
G. M. Schneider
Aqueous solutions at pressures up to 1.5 GPa: Gas-gas equilibria, closed loops, high-pressure immiscibility, salt effects and related phenomena

S. Raeissi, C. J. Peters
On the phenomenon of double retrograde condensation

C. E. Schwarz, I. Nieuwoudt
Phase equilibria for synthetic wax fractionation

A. L. Scheidgen, G. M. Schneider
New phase phenomena in ternary systems at high pressures – cosolvency and miscibility windows up to 100 MPa

Tuesday, August 21
Morning I, 8.45-10.30
G. Maurer (*invited*)
Phase equilibrium of hydrogel systems

J. Salminen, O. Antson
Physico-chemical modeling and experiments involving reactive aqueous solution

A. Toikka
Topological analysis of phase diagrams for reactive systems

S. Blagov, H. Hasse
Topological analysis of phase diagrams for distillation process design

Morning II, 11.00-12.25
C. Vega, C. McBride, L. G. MacDowell (*invited*)
Complex fluids, simple models

M. Y. Nagamachi, A. Z. Francesconi
Molecular modeling of phase equilibria properties G^E and H^E of aqueous systems containing alkanediols

F. Aicardi, P. Valentin, E. Ferrand
On the classification of generic phenomena in thermodynamic binary mixtures models depending on parameters

Afternoon I, 14.00-15.45
D. A. Kofke (*invited*)
Molecular modeling and applications of phase transitions in solids

T. Kuznetsova, B. Kvamme
Pure molecular-dynamics grand canonical treatment for water and methanol model systems

R. Kohli
Thermodynamics and phase diagrams of binary supercritical CO_2 mixtures for application in precision cleaning

Afternoon II, 16.15-17.45
T. Boublík
Phase equilibria in supercritical fluid extraction. Systems of the Kihara molecules

E. J. M. Filipe, L. M. B. Dias, J. C. G. Calado, C. McCabe, G. Jackson
Is xenon an “ennobled” alkane?

R. J. Sadus
An alternative to the “hard-sphere + attractive term” approach for equations of state for fluids and fluid phase equilibria

Wednesday August 22
Morning I, 8.45-10.30
J. F. Brennecke, M. A. Stadtherr (*invited*)
Reliable computation of phase behavior using interval analysis

B. Dąbrowska
Prediction of the thermodynamic properties of the new alternative refrigerants (halogenhydrocarbons /hydrocarbons mixtures) on the base of the equations of state

G. Silva-Oliver, L. A. Galicia-Luna, S. I. Sandler
Vapor liquid equilibria near critical point and critical points for the CO_2+1-hexanol and CO_2+1-heptanol systems at temperatures from 324 to 434 K

I. Goodarznia, F. Esmaeilzadeh
Solubility of anthracene, phenanethrene and carbazole mixture in supercritical carbon dioxide

Morning II, 10.50-11.50
A. Oleinikova, I. Brovchenko, A. Geiger, B. Guillot,
Percolation of water and liquid-liquid immiscibility of aqueous solution

J. N. A. Canongia Lopes
Microphase separation in model racemic mixtures

I. Polishuk, J. Wisniak, H. Segura
Transitional behavior of phase diagrams predicted by semi-empirical cubic equations of state and classical mixing rules.

Poster Presentations
Monday, August 20, 20.00-22.00

1. A. Oleinikova, H. Weingärtner (p 67)
Pecularities of the liquid-liquid phase behavior in aqueous solutions: Novel phase on the meniscus and effect of distant critical point on the shape of coexistence curve.

2. I. Goodarznia, F. Esmaeilzadeh (p 68)
A new special design for the equilibrium cell for measuring the solubility of organics in supercritical carbon dioxide."

3. H. Ruf, E. Lewitzki, E. Grell, R. Schneider, G. Ilgenfritz (p 69)
Nonionic detergent micelles: growth and changes in structure associated with a thermal transition

4. S. Enders, A. R. Imre, A. Stammer, B. A. Wolf (p 70)
On the effect of polydispersity on the cloud point curve of a binary blend consisting of polyalkylsiloxanes

5. M. M. Mooijer – van den Heuvel, C. J. Peters (p 71)
Systematic study on gas hydrate phase equilibria of systems of methane, propane, carbon dioxide and nitrogen in the presence of pressure-reducing agents

6. Z. P. Visak, R. G. de Azevedo, L. P.N. Rebelo, J. Szydlowski , H. C. de Sousa, V. Najdanovic-Visak (p 72)
Double critical phenomena in aqueous polyacrylamides solutions

7. D. Tůma, B. Wagner, G. M. Schneider (p 74)
Temperature, pressure, and density dependencies of the solubilities of low-volatile organic dyestuffs in compressed gases

8. M. Roth, K. Maag, G. M. Schneider, D. Tůma (p 75)
Partial molar properties and solute–solvent interactions in dilute solutions of C_{60} and C_{70} fullerenes and C_{21} to C_{40} *n*-Alkanes in CO_2 from supercritical fluid chromatography

9. J. T. Safarov (p 76)
Thermodynamic properties of methanol + water solutions from the "liquid - vapor" phase transition line up to 60 Mpa

10. A. Shahverdiyev (p 77)
P-ρ-T and P_s-ρ_s-T_s dependence of vapor aqueous solutions of propyl alcohol

11. E. Roduner, G. Zhao, B. Groß, H. Dilger (p 78)
Calorimetric properties of an interconnected array of clusters of benzene adsorbed on NaY zeolite