



Thermochemical, Thermodynamic, and Transport Properties of Halogenated Hydrocarbons and Mixtures

Poster presented at the
IUPAC Congress/General Assembly
July 2001

Aims

To improve our knowledge and understanding of thermodynamic and transport properties for these compounds and mixtures in the fluid state.

This is of industrial importance because these fluids find application:

- as solvents
- as refrigerant and air-conditioning fluids
- as foam-blowing agents
- as artificial oxygen carriers, and in liquid ventilation
- as fluoruous media for biphasic catalysis

Workshop, Paris 2001

The purpose of this workshop - with 11 invited lectures, 27 oral and 59 poster presentations, and a round-table discussion - was

- to consider environmental constraints and regulations
- to present and discuss new experimental measurements, particularly for the systems:
 - propane/butane + refrigerants
 - binary and ternary HFC mixtures
 - higher alkanes/ethers + fluoroalkanes
 - lubricant oils + refrigerants
 - gas + perfluorocarbons, with medical application

- to present and discuss the results of calculation, particularly:
 - intermolecular potential calculations for methane-, ethane- and propane-derived HCFCs and HFCs using *ab initio* methods, to develop models for calculation of macroscopic properties
 - molecular simulations, especially for methane derivatives
- to present and discuss improved correlation methods

Invited lectures

Environmental issues:

Actions in the European Union against ozone depletion and climate change: impacts on the refrigeration and air-conditioning industries.....N. Campbell, ATOFINA

EC policy on protecting the ozone layer - the new regulationP. Horrocks, European Commission

Refrigerants and air-conditioning:

Fluorocarbons in refrigeration and air-conditioning: main options of the French national program ..C. Ewald, M.A.T.E.

Are we near an industry standard for refrigerant properties?
.....D.B. Bivens and J.R. Morley, DuPont Fluoroproducts

Thermodynamic properties:

Halogenated hydrocarbons: selected thermodynamic aspects
.....E. Wilhelm, University of Vienna

High pressure phase equilibrium and spectroscopic investigations
up to 200 MPa on binary mixtures containing a fluorinated
compound, an ether, an inert gas, an alkane, or a selected polar
substance: review and new results.... G.M. Schneider, Bochum

Phenomenology of high-pressure phase behavior of systems
containing halocarbons.....Th.W. de Loos, Delft

Electrical characterization of ten binary and ternary alternative
refrigerant mixtures....A.Laesecke and R.F. Hafer, NIST, USA

Thermodynamic properties of binary HFC + HC refrigerants
Y. Kayukawa, S. Naganuma, and K. Watanabe, Keio Univ.,
Japan

Computations:

The use of computational chemistry to predict the phase
behaviour of complex systems.....S.I. Sandler, Univ. of Delaware

Correlation methods:

Advanced development of the corresponding states modeling
techniques in the three-parameter format. Applications to
refrigerants.....G. Scalabrin, Universita di Padova, Italy

Selected Oral Presentations

A decade of progress in calorimetry: HFCs and their mixtures
.....J.W. Magee, NIST, Boulder, USA

Thermodynamics of refrigerants plus lubricant oils.....
K.N. Marsh and M. Kandl, Univ. of Canterbury, New Zealand

Prediction of thermophysical properties of mixtures of
alternative refrigerants by molecular simulations.....
M. Fermeglia, O. Milocco, and S. Prigl, Univ. of Trieste, Italy

On the correlation of transport properties of liquid mixtures...
M.J. Assael, N.K. Dalaouti, and I. Metaxa, Thessaloniki, Greece

VLE measurements and modeling for the strongly positive
azeotrope R32 + propane system.....S. Bobbo, L. Fedele, and
R. Camporese, Padova, Italy and R. Stryjek, Warsaw, Poland

Publications

Two Workshops have been held as part of this project. The Workshop Proceedings are published as Special Issues of *Fluid Phase Equilibria*:

1st International Workshop, Pisa, Italy, Dec. 15-18, 1999 in *Fluid Phase Equilibria*, Vol. 174 (2000), 1-246

2nd International Workshop, Paris, France, April 9-11, 2000, *Fluid Phase Equilibria*, to be published.

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