SECOND INTERNATIONAL WORKSHOP ON THERMOCHEMICAL, THERMODYNAMIC, AND TRANSPORT PROPERTIES OF HALOGENATED HYDROCARBONS AND MIXTURES

Paris, France

April 9–11, 2001

This is the second in a series of workshops held under the auspices of the IUPAC, International Union of Pure and Applied Chemistry, Commission on Thermodynamics. The objective of this project is to increase our knowledge and understanding of thermodynamics and transport properties of halogenated organic compounds, especially halogenated aliphatic hydrocarbons, of their mixtures, and of mixtures with hydrocarbons. This has an important industrial application in the widespread use of these substances as solvents, refrigerants, blood substitutes, foam-blowing agents, fire extinguishers, insulation in high-voltage switches, and surfactants for extraction processes involving supercritical carbon dioxide. Further information about the project is available at http://www.iupac.org/projects/1998/121_18_98.html.

Main Themes of the Workshop

1. Environmental constraints and regulation
2. New products (refrigeration, medicine, insulators, etc.)
3. New measurements, physical property characterization
4. Fundamentals (intermolecular potentials with O, F, and Cl as the main heteroatoms of interest) and simulation

AIMS OF THE WORKSHOP

(1) To present and discuss new experimental measurements, particularly for the systems

- Propane/butane + refrigerants
- Binary and ternary HFCs
- Higher alkanes/ethers + fluoroalkane
- Lubricant oils + refrigerants
- Gas + perfluorocompounds, with medical application

(2) To present and discuss the results of calculations, particularly

- Intermolecular potential calculations for methane-, ethane-, and propane-derived HCFCs using *ab initio* methods, to develop models for theory-based calculation of macroscopic properties
- Molecular simulations, particularly for methane derivatives
- Improved correlation methods

(3) To review progress and to recommend topics for experimental and theoretical studies to be carried out for presentation at the final workshop in 2002

Sessions will comprise invited lectures, short communications, posters, poster discussion, and a panel round-table discussion.

Further information about the workshop (including deadlines for submission of contributions and registration fees) is available at the website: http://www-cenerg.ensmp.fr/iupac_paris.wshop.

Contact

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Printed in Belgium