



Introduction to the special issue of the Journal of Molecular Liquids "Supercritical fluids. Theory and applications" dedicated to Prof. Yu. E. Gorbaty

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Abdenacer Idrissi, M.G. Kiselev, Andrey G. Kalinichev. Introduction to the special issue of the Journal of Molecular Liquids "Supercritical fluids. Theory and applications" dedicated to Prof. Yu. E. Gorbaty. Journal of Molecular Liquids, 2017, 239, pp.1-2. 10.1016/j.molliq.2017.05.073 . in2p3-01577628

HAL Id: in2p3-01577628

<https://hal.in2p3.fr/in2p3-01577628>

Submitted on 9 Oct 2018

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Editorial

Introduction to the special issue of the *Journal of Molecular Liquids* “Supercritical fluids. Theory and applications” dedicated to Prof. Yu. E. GorbatyAbdenacer Idrissi^{a,*}, Mikhail G. Kiselev^b, Andrey G. Kalinichev^c^a Université des Sciences et Technologies de Lille, France^b Institute of Solution Chemistry of the Russian Academy of Sciences, Ivanovo, Russia^c Laboratoire SUBATECH (UMR 6457), Institut Mines-Télécom Atlantique, Nantes, France

ARTICLE INFO

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Article history:

Available online xxx

Professor Yuri E. Gorbaty was born 30 July 1932 in the city Grozny, in the Soviet Union. He has graduated from the Mendeleev Institute of Chemical Technology, Moscow, in 1955. He has got his Candidate of Sciences (Ph.D.) degree in 1963 for his work on “Non-equilibrium crystallization of the three-component melts”, and later in 1988 he was awarded a Doctor of Sciences degree for the work “The effect of temperature and pressure on the nearest ordering in liquid and supercritical water”. Between these two dates and then later in his scientific career Yuri E. Gorbaty has become one of the leading experts in the field of experimental studies of the structure and properties of fluids, especially aqueous fluids at high temperatures and pressures, by methods of IR and Raman spectroscopy and by X-ray diffraction.

The uniqueness of his approach to the studies of hydrothermal solutions was in the simultaneous application of several complementary methods to investigate the same object under the same set of thermodynamic conditions. He has devoted a lot of efforts to develop a range of very original and sophisticated experimental optical and X-ray diffraction cells that could reliably withstand extreme conditions of hydrothermal experiments, while still allowing optical and X-ray access to the fluid sample inside through very cleverly designed and carefully sealed windows [2,13,18,24–27,29,38,46]. Particularly interesting and effective is the IR cell, the thickness of the absorbing layer in which can vary within a range of 0–1.5 mm directly during the experiment at high temperatures (up to 550 °C) and pressures (up to 1500 bars) with an accuracy of $\pm 0.5 \mu\text{m}$ [24]. In the cell for Raman spectroscopy with internal vessels, the fluid sample only contacts with sapphire and gold, which avoids any interaction of the metal walls of the high-pressure cell with highly corrosive supercritical solutions [45]. Cells for energy dispersive X-ray diffractometry, UV spectroscopy and many other devices were also created for

conducting physical experiments at high temperatures and pressures [27,46].

The most valuable data were obtained by measuring the intensity of X-ray scattering from water up to $t = 550 \text{ }^{\circ}\text{C}$ and $P = 1000 \text{ bar}$ and up to 8000 bar at room temperature and for the first time extracting experimental information about molecular pair correlation functions of water under these extreme conditions [14–17,19,20,28]. These data were complemented by the results of studies using infrared absorption spectroscopy and Raman scattering [4–5,8–9,23,31,38–39].

Yu.E. Gorbaty proposed a new approach to the description of the structure of liquid and supercritical water, based on the percolation theory. It was shown that the liquid and supercritical states differ qualitatively depending on the existence or absence of an infinite cluster of hydrogen-bonded molecules [33,34]. The percolation threshold for a three-dimensional network of hydrogen bonds in water is reached in the region of the critical isotherm. Below the percolation threshold, only clusters of finite size can exist in the supercritical region. This explains many interesting and still misunderstood phenomena that occur during the transition of a liquid to the supercritical state. One of the brilliant findings of Prof. Gorbaty together with his colleagues was the experimentally proven idea of universality of hydrogen bonding behavior of alcohols under supercritical conditions [44]. Until his last days, he was always full of new ideas, and was always ready to share them with his colleagues.

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