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The Editorial Board "Supercritical Fluids: Theory and Practice"

The 10th Scientific and Engineering Conference with International Participation "Supercritical Fluids: Fundamentals, Technologies, Innovations"

BOOK of ABSTRACTS

30 September 2019 - 06 October 2019 Rostov-on-Don

Don-2019

CONDUCTING NMR EXPERIMENTS AT SUPERCRITICAL PARAMETERS OF STATE

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NMR spectroscopy is an indispensable method for analyzing the structure and dynamics of molecules in liquids. Modern NMR approaches allow obtaining direct information about the geometrical configuration of molecules in liquids, which is very important when solving problems of modern physical chemistry of fluids. However, the NMR method is extremely problematic when it touches upon experiments at pressures above 100 bar. This report presents the peculiarities of a high pressure NMR experiment, as well as the effect of the NMR cell on the resolution of the spectrometer. In addition, the latest results obtained using the unique molecular fluid spectroscopy instrumentation at G.A. Krestov Institute of Solution Chemistry will be presented and discussed together with the development vistas and possibilities of this method.

The experimental data were obtained using the molecular fluid spectroscopy facility of G.A. Krestov Institute of Solution Chemistry, RAS.

The work was supported by the Ministry of Science and High Education of the Russian Federation (project number: RFMEFI61618X0097)

[1] Khodov I.A., Dyshin A.A., Ivlev D.V., Kiselev M.G., High pressure NMR spectroscopy technique as applied to conformational equil ibrium research of small druglike molecules at supercritical conditions, VIII Scientific and Practical Conference with international participation "Supercritical Fluids (SCF), 2017, 199.