

Russian Academy of Sciences

Russian Foundation for Basic Research

Southern Federal University

G.A. Krestov Institute of Solution Chemistry of the Russian Academy of Sciences

N.S. Kurnakov Institute of General and Inorganic Chemistry of the Russian Academy of Sciences

Federal Research Center "Crystallography and Photonics" of the Russian Academy of Sciences

M.V. Lomonosov Moscow State University

ZAO "Schag"

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

INVESTIGATION OF THE MOLECULAR STRUCTURE OF MEFENAMIC ACID IN SUPERCRITICAL CARBON DIOXIDE BY TWO-DIMENSIONAL NMR SPECTROSCOPY

Khodov I.A.^{1,2}, <u>Belov K.B.</u>¹, Dyshin A.A.¹, Efimov S.V.², Kiselev M.G.¹

¹G.A. Krestov Institute of Solution Chemistry of Russian Academy of Sciences, Ivanovo, Russian Federation

²Institute of Physics, Kazan Federal University, Kazan, Russian Federation iakh@isc-ras.ru

Polymorphism of biologically active compounds is a serious problem for the pharmaceutical industry because of its effect on the physical and chemical properties of solid powders. Therefore, the control of the polymorphism of medicinal compounds is a very important and urgent task. The compound possessing conformational polymorphism was chosen as the object of the study (mefenamic acid). Polymorphic forms of mefenamic acid show an enantiotropic transition, the transformation of form I into form II occurs at temperatures above 180°C [1]. Hence, a possible conversion to form II (metastable form) may jeopardize the stability of a pharmaceutical product and may change the effectiveness of the drug. Since the forms of mefenamic acid are determined by the molecular structure, it becomes necessary to investigate its structure in a critical state. This information will help to identify the nature of the nucleation of mefenamic acid. In the present work, the molecular structure of mefenamic acid was studied at supercritical state parameters by two-dimensional NMR spectroscopy.

The experimental data were obtained using the molecular fluid spectroscopy facility of G.A. Krestov Institute of Solution Chemistry, RAS (unique scientific equipment no. 503933). The reported study was funded by the Russian Foundation for Basic Research according to the project no. 18-03-00255. Partial funding was provided by a grant from the President of the Russian Federation for state support of young Russian scientists – candidates of sciences: MK-1409.2019.3.

 Khodov I.A., Belov K.V., Efimov S.V., Batista de Carvalho L.A.E. Determination of preferred conformationsof mefenamic acid in DMSO by