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ABSTRACTS

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High-pressure NMR Characterization of Conformation Preferences of Small-Molecules Dissolved in Supercritical Carbon Dioxide

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The application of this approach to the study of conformational preferences in a fluid seems very promising in relation to obtaining information on the processes occurring at the molecular level. One of the key tasks for obtaining this kind of information is adapting NMR methods for high temperatures and pressures.

High-pressure NMR spectroscopy has been utilized to study the conformation behavior of small molecules dissolved in supercritical CO_2. The 2D NOESY spectrum was analyzed to determine the conformation preference. A change in the conformation distribution is postulated to describe the nucleation mechanism of different polymorphic forms. At the CO_2 supercritical parameters of state, there is an apparent coincidence conformation preference of the small molecules in fluid volume and in solid phase. This fact is confirmed by the results of computer simulation.

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[1] I.A. Khodov, S.V. Efimov, V.V. Klochkov, L.A.E. Batista De Carvalho, M.G. Kiselev, J. Mol. Struct., **1106**, 373 (2016).
[2] S.V. Efimov, I.A. Khodov, E.L. Ratkova, M.G. Kiselev, S. Berger, V.V. Klochkov, J. Mol. Struct., **1104**, 63 (2016).