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Book of
ABSTRACTS

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An Investigation of the Conformational Properties of Mefenamic Acid in DMSO by Two-dimensional NMR

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This abstract presents the main results of research on the conformational preference of the molecule mefenamic acid. This compound is used as a drug and belongs to the group of NSAID (nonsteroidal anti-inflammatory drugs). The main idea of this research is to determine the conformation preference of mefenamic acid dissolved in deuterated DMSO using two-dimensional NMR and quantum chemistry calculation. The obtained information can help one to determine the way of nucleation mechanisms.

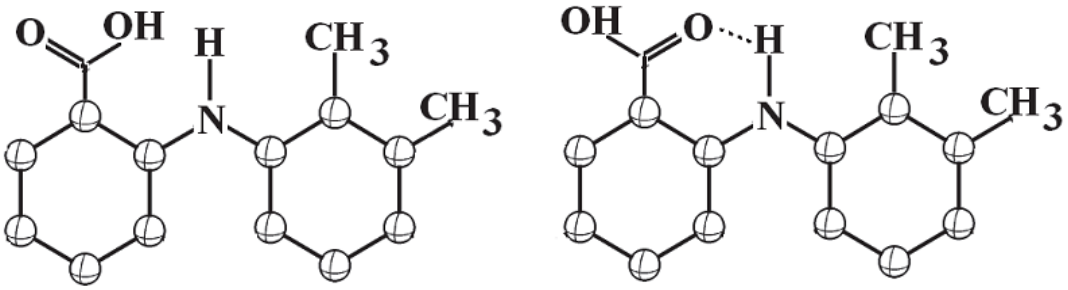

Figure 1. Structure of the mefenamic acid polymorphs molecules MEF II (left) and MEF I (right).

Two crystalline forms, called MEF I and MEF II, having different positions of the carboxyl group, are formed by different conformations of the mefenamic acid molecules (Fig.1)[1].

Recently we have shown that the molecular conformation, existing in the saturated solution, may define the polymorphic type, obtained by evaporation of this solution [2,3].

In this work we present the conformation equilibrium of mefenamic acid in solution and discuss it in the frame of polymorphic phenomena.

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