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Theoretical studies of Mefenamic Acid Polymorphs: Solid-state ^{13}C carbon-NMR and vibrational (IR and Raman) Spectroscopies.

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The two polymorphs of mefenamic acid (MEF) or 2-[(2,3-(dimethylphenyl)amino] benzoic acid polymorphs (known as I and II forms) were studied in the framework of density functional theory (DFT). The DFT calculations were performed using the Gaussian03 package [1] and these results were compared with experimental data of solid-state ^{13}C Nuclear Magnetic Resonance (NMR), vibrational Raman and infrared spectroscopies. The molecules arrangements are centrosymmetric dimmers over the eight-membered ring formed by the two carboxylic groups for both polymorphs. ^{13}C NMR data pointed out differences between both polymorphs by three major groups: carboxylic, aromatic ring and methyl group. The ^{13}C chemical shifts for the dimethylphenyl group are quite dissimilar for forms I and II and the Raman band related to the C-N stretching is the most sensitive mode in both MEF conformation. Hence the spectral analysis of mefenamic acid polymorphs conducted in this work lead to NMR peaks and vibrational bands that identify these polymorphs. The vibrational data of MEF II supported by DFT calculations are reported by the first time in this study, as well as, the solid state ^{13}C NMR spectra of MEF I and MEF II compounds.

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[1] Frisch, M.J. et al. *Gaussian 03, Revision A.1*, Gaussian Inc., Pittsburgh, PA,(2003).

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