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Investigating ketoprofen using experimental methods and quantum chemical modeling

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A study of ketoprofen was carried out using experimental as well as computational methods. Ketoprofen is a representative of the group of non-steroidal anti-inflammatory drugs widely used in modern medical therapy. It has a high analgesic, anti-inflammatory and antipyretic activity. Reactivity of ketoprofen is closely connected with its structures features. Ketoprofen sample was investigated by the following experimental methods: differential scanning calorimetry, IR-spectroscopy and Raman-spectroscopy. The structure of ketoprofen was also investigated by DFT (BP86/def2-SVP) method. A comparative analysis of the calculated and experimental data was performed. Investigation of ketoprofen sample by IR spectroscopy demonstrated concordance of spectra obtained in KBr tablet and by FTIR method. The most intensive peaks in these spectra correspond to the ν(C-O) and two ν(C=O) vibrations. A good agreement between the experimental and calculated in the DFT approximation vibrational frequencies of ketoprofen was obtained.

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