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Structure and dynamics investigation of ibuprofen dimers by DFT method.

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Ibuprofen is a representative of the group of non-steroidal anti-inflammatory drugs widely used in modern medical therapy. The drug formulations of Ibuprofen most often contain a racemic mixture of the two enantiomers with the S enantiomer being biologically active and the R being inactive. Cyclic dimers of Ibuprofen can be distinguished in condensed state of this compound that is confirmed by X-ray diffraction analysis. In solvent the formation of dimers with other configurations can be expected: linear and/or cyclic associates with another type of binding. The presence of such dimers will influence the vibrational dynamics of ibuprofen in condensed matter.

The object of present study is ibuprofen enantiomers and their dimers. Both enantiomers (S and R) were taken into account when constructing dimer models. The combination of computational (DFT) and experimental (IR and Raman spectroscopy) methods were used in the study.

For all the dimers studied, the parameters of molecular geometry and characteristics of hydrogen bonding were calculated and analyzed. The strength of the hydrogen bond and the stability of ibuprofen dimers are discussed. It has been shown that the presence of an intermolecular hydrogen bond affects the vibrational frequencies of groups of atoms involved in intermolecular interactions (the carboxyl group). This gives more correct results comparable to the experiment.

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