

State of water in various environments: Aliphatic ketones. MIR/NIR spectroscopic, dielectric and theoretical studies

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Streszczenie

This work provides new insight into the state of water in a series of aliphatic ketones. For our studies, we selected nine aliphatic ketones of different size and structure to examine the effect of various structural motifs on behavior of water in the mixtures. Our results reveal that conformational flexibility of aliphatic chains in the linear ketones allows for effective shielding of the carbonyl group, and this flexibility is the main reason for poor solubility of water. Hence, in the linear ketones molecules of water are involved mostly in ketone-water interactions, while the water-water interactions are rare. Higher solubility of water in the cyclic ketones allows for creation of clusters of water, where the molecules are in water-like environment. The temperature rise in wet cyclic ketones increases population of ketone-water interactions at the expense of the water-water ones, while in the linear ketones and 2,6-dimethylcyclohexanone at an elevated temperature there is an increase in the population of singly bonded water at the expense of the doubly bonded one. DFT calculations reveal that the substitution of cyclohexanone by a single methyl group does not affect the strength of the ketone-water interactions, while it has a significant impact on the solubility of water in the ketone. The most important conclusion from this study is that the accessibility of the carbonyl group is the most important factor determining the intermolecular interactions and solubility of water in aliphatic ketones.

Słowa kluczowe

Ketones, Water, Binary mixtures, Hydrogen bonding, Intermolecular interactions, Solubility, MIR/NIR spectroscopy, Liquids, Molecular structure

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