

Microheterogeneity in CH₃OH/CD₃OH mixture.

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Recently, we demonstrated the presence of microheterogeneity in binary mixtures of unlike alcohols. [*RSC Adv.* 2016, 6, 37195–37202] The aim of this work was examination if this phenomenon occurs also in the mixture of very similar alcohols like CH₃OH and CD₃OH. Theoretical calculations suggest that the isotopic substitution in methyl group influences properties of the OH group. Hence, one can expect that this effect may lead to partial separation of CH₃OH and CD₃OH at a molecular level and it contributes to deviation from the ideal mixture. This work evidences that CH₃OH/CD₃OH mixture also deviates from the ideal one, but the extent of this deviation is much smaller as compared with the mixtures of other alcohols. It is of particular note that this deviation results mainly from the difference between the CH₃ and CD₃ groups, while the contribution from the OH groups is small. The structure of CH₃OH/CD₃OH mixture at a molecular level is similar to the structure of binary mixtures of other alcohols. The mixture is composed of the homoclusters of both alcohols and the mixed clusters. The homoclusters existing in the mixture are similar to those present in bulk alcohols. The highest population of the heteroclusters and the largest deviation from the ideal mixture were observed at equimolar mixture. Both the experimental and theoretical results reveal that in CH₃OH/CD₃OH mixture dominate the cyclic tetramers and larger clusters, while the population of the linear clusters is negligible. Though the extent and strength of hydrogen bonding in both alcohols are the same, the position and intensity of the 2ν(OH) band for CH₃OH and CD₃OH are different. We propose possible explanation of this observation

Słowa kluczowe

Binary mixtures, Methanol, Methanol-d3, Liquid phase, Molecular structure, Microheterogeneity, hydrogen bonding, spectroscopy, aTR-IR, nIR, 2D correlation analysis, chemometrics, MCR-ALS, Excess spectra, density functional theory

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