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Influence of Environment on Vibrational Spectra of Hydrogen-Bonded Clusters

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Quantum-chemical calculations (by DFT method in B3LYP/cc-pVTZ approximation) of optimal structure and vibrational spectra of water and methanol clusters in different media were carried out using Gaussian 09 software. Water clusters consisting of from one to six molecules in vacuum, water and argon media were considered. By comparison of the calculated IR absorption spectra of clusters in different media it is shown that the environment affects the spatial structure of hydrogen-bonded clusters of water molecules, and this influence is manifested in the shifting of the vibrational bands.
Similar calculation was made for methanol clusters (monomer, dimer, trimer) in vacuum, methanol, water and argon. Different shifts for different media were observed. It is shown that the influence of argon is greater than the influence of methanol.
The calculated IR absorption spectra of water and methanol clusters in different environments were compared with the corresponding spectra in vacuum, and so the spectral shifts for all IR bands were determined. The determined spectral shifts can be considered as matrix shifts observed during the experimental study of alcohol and water clusters in low-temperature argon matrices. In particular, it is shown that the presence of argon has a stronger effect on the structure of methanol clusters than their surrounding by methanol molecules, so the vibrational spectra of methanol in matrix isolation will be different from the vibrational spectra of methanol in a liquid or gaseous state.

Topics

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