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Effect of a low-temperature Ar matrix on hydrogen-bonded clusters (H2O)n

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Matrix isolation is one of the most effective methods to investigate individual molecules of small clusters by spectroscopic methods. Though the matrix material is inert, there is still an effect of low-temperature matrices on the structure and vibrational spectra of isolated molecules. The main purpose of this study is to investigate the argon matrix effect on the structure, dynamics, and infrared (IR) spectra of small water clusters $(H_2O)_n$ with n = 1 - 6. Quantum-chemical calculations of optimal structure and IR spectra of the mentioned clusters in a face-centered cubic (fcc) argon crystal fragment with 108 Ar atoms were made using Gaussian software. The calculations were carried out by the M06-2X method with CRENBL EC basic set for Ar atoms and aug-cc-pVD basic set for water molecules. The results of calculations were compared to the experimentally registered IR spectra of water clusters in an Ar matrix and the corresponding assignment of the spectral band was made.

Topics

Session A. Physics of condensed matter and spectroscopy

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