

## QUANTUM-CHEMICAL ACCOUNT OF IR SPECTRA HYDRATED CATIONS

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With use of the program Gaussian 03 the influence of a method of account and basis on IR spectra of a molecule of water, dimer of water and hydrated by one and two molecules of water cations of alkaline metals ( $\text{Li}^+$ ,  $\text{Na}^+$ ,  $\text{K}^+$ ,  $\text{Rb}^+$ ) is investigated.