THEORETICAL STUDY OF THE OH/OD STRETCHING REGIONS OF THE VIBRATIONAL SPECTRA OF ICE IH

M.J. WÓJCIK, K. SZCZEPONEK, *Faculty of Chemistry, Jagiellonian University, 30-060 Kraków, Ingardena 3, Poland*; S. IDEDA, *Neutron Science Laboratory, High Energy Accelerator Research Organization, Tsukuba, Ibaraki 305-0801, Japan*.

In this paper we present results of our theoretical studies of the vibrational spectra of ice Ih in the stretching mode frequency range. They include simulation of the infrared and Raman spectra for the OH and OD stretching regions, the effects of a full range of isotopic dilution on the spectra (including polarized Raman spectra) and computational modeling of the observed influence of each dilution step on the properties of vibrationally excited states and on the infrared and Raman spectra. In our calculations we included effects of frequency lowering due to hydrogen bonding, and of intra- and intermolecular coupling between bonds. In the crystalline isotopomers the properties of the vibrationally excited states and of the spectra are determined by a complex interplay between the size distributions of the embedded clusters and the inter- and intramolecular couplings.