HIGH RESOLUTION INFRARED SPECTROSCOPY OF WATER MONOMERS AND WATER CLUSTERS IN SOLID PARAHYDROGEN

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I report on progress made in assigning the various infrared (IR) absorption features observed in the spectra of water-doped cryogenic molecular hydrogen solids. Since water is a ubiquitous impurity in our samples, this ”cataloging” stage is a prerequisite to correctly identifying the IR absorptions due to other dopant species of interest. The water assignments are complicated by a number of phenomena, including: (1) clustering of H_2O molecules, (2) clustering of residual ortho-H_2 molecules with water molecules and clusters, and (3) the surprisingly rapid ortho/para conversion of H_2O and D_2O molecules, both isolated and in clusters. A few highlights: (a) H_2O, D_2O, and HDO monomers all exist as very slightly hindered rotors in para-H_2 solids, (b) clustering of these monomers produces novel non-minimum-energy water cluster configurations such as the cyclic water hexamer reported in J. Chem. Phys. v115, p6807 (2001), (c) clustering of water monomers with residual ortho-H_2 yields spectra of ”non-rotating” water molecules and as-yet un-assigned complex spectra presumably due to ortho-H_2/water van der Waals clusters, and (d) the ortho-to-para H_2O and para-to-ortho D_2O conversion of isolated monomers both follow single-exponential decay profiles with time constants of 1900 s and 860 s, respectively.