

OVERTONE VIBRATIONAL SPECTROSCOPY AND DYNAMICS IN H₂-H₂O COMPLEXES: A COMBINED THEORETICAL AND EXPERIMENTAL STUDY

MICHAEL P. ZIEMKIEWICZ, CHRISTIAN PLUETZER, DAVID J. NESBITT, *JILA, University of Colorado and National Institute of Standards and Technology, Boulder, Colorado*; YOHANN SCRIBANO, *CNRS-Université de Bourgogne, Dijon, France*; ALEXANDRE FAURE, *CNRS, Institut de Planétologie et d'Astrophysique de Grenoble(IPAG), France*; AD VAN DER AVOIRD, *Radboud University, 6525 AJ Nijmegen, The Netherlands*.

H₂ is the most abundant molecule in the universe and also H₂O occurs in relatively high concentrations in various interstellar environments. Processes that occur through the interaction of these molecules may, for example, play a role in the mechanism producing the observed H₂O maser activity. Spectroscopic studies of the H₂-H₂O complex in different stable and metastable states will be reported in the accompanying talk; theoretical studies will be presented here. The latter involve calculations of the bound rovibrational levels of the complex with both monomers in their vibrational ground state, as well as of the metastable levels with H₂O in its OH stretch overtone state, on the appropriate *ab initio* five-dimensional intermolecular potential surfaces. Also the line strengths of all the allowed transitions between these levels that may occur in combination with the $v_{\text{OH}} = 2 \leftarrow 0$ overtone transition were computed, for all four ortho/para H₂ and ortho/para H₂O variants of the complex. The spectrum simulated with these data agrees very well with the measured spectrum and was used to assign this spectrum. In addition, the information obtained from the theory was useful to understand the observed predissociation dynamics of the complex.