THE IUPAC CRITICAL EVALUATION OF THE RO-VIBRATIONAL SPECTRA OF WATER VAPOR: RESULTS FOR $H_2{}^{18}O$, $H_2{}^{17}O$, AND $HD^{16}O$

J. TENNYSON, *University College London, Department of Physics and Astronomy, London, UK*; A. G. CSÁSZÁR, T. FURTENBACHER, *Loránd Eötvös University, Institute of Chemistry, Budapest, Hungary*; A. Z. FAZLIEV, *Institute of Atmospheric Optics, RAS, Tomsk, Russia*; I. E. GORDON, L. S. ROTHMAN, *Harvard-Smithsonian Center for Astrophysics, Atomic and Molecular Physics Division, Cambridge MA 02138-1516, USA*.

A water-vapor task group was recently formed under the sponsorship of the International Union of Pure and Applied Chemistry (IUPAC). The group is comprised of 14 members from the international community, representing expertise in theory, experiments, and data handling. The goal of this task is to create a compilation of quality experimental and observational data pertaining to water vapor at both room temperature and high temperature. This task includes a critical evaluation of line positions, energy levels, line intensities, and line-shape parameters for all of the major isotopologues of the water molecule. The spectral coverage is from the microwave through the visible.

The first results have been obtained for the three isotopologues $H_2{}^{18}O$, $H_2{}^{17}O$, and $HD^{16}O$. The initial focus was on obtaining critically evaluated, self-consistent sets of energy levels, and these isotopologues were chosen prior to engaging the principal isotopologue, for which there is a much more abundant dataset.

The IUPAC database also will employ the methodology of relational databases to store and retrieve both theoretically-determined parameters as well as experimental. In this sense, it may serve as a paradigm for databases such as HITRAN.