

ANALYSIS OF NEW DATA SETS PERTAINING TO THE WATER MOLECULE

S. YU, J. C. PEARSON, B. J. DROUIN, *Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA 91109, USA*; H. S. P. MÜLLER, S. BRÜNKEN, *I. Physikalisches Institut, Universität zu Köln, 50937 Köln, Germany*; M. A. MARTIN-DRUMEL, O. PIRALI, D. BALCON, M. VERVLOET, *Ligne AILES – Synchrotron SOLEIL, L’Orme des Merisiers, Saint Aubin, 91192 Gif-sur-Yvette, France*; AND L. H. COUDERT, *LISA, CNRS/Universités Paris Est et Paris Diderot, 61 Avenue du Général de Gaulle, 94010 Créteil, France*.

Although water is just a simple triatomic molecule, its spectroscopy still remains a challenge due to the ever increasing amount of available data. Two types of data have been recently obtained for water:

- Accurate frequencies have been measured for transitions in the sub millimeter and terahertz domains involving high-lying rovibrational levels up to the first triad. 149 transitions have been measured between 300 GHz and 2 THz and 26 from 2.5 to 2.7 THz. These *b*-type transitions take place within one of the five first vibrational states.
- Far infrared transitions involving high-lying rovibrational levels have been recorded recently in the 50 to 600 cm^{-1} region using the emission spectrum of a continuous flow of water vapor rovibrationally excited by an electrodeless radio-frequency discharge.^a 3793 transitions with $\Delta K_a = 1$ within one of the five first vibrational states of the molecule have been assigned so far and involve *J*-values up to 25 and *K_a*-values up to 15. There remains a large number of unassigned transitions involving either higher lying vibrational states, larger values of ΔK_a , or taking place between different vibrational states.

The paper will focus on the results of the analysis of a large data set consisting of already published data^b and of the two new data sets. The number of data is equal to 20491 and the bending-rotation theoretical approach^c will be used for the energy level calculation.

^aPirali and Vervloet, *Chem. Phys. Letters* **423** (2006) 376.

^bCoudert, Wagner, Birk, Baranov, Lafferty, and Flaud, *J. Molec. Spec.* **251** (2008) 339.

^cCoudert, *J. Molec. Spec.* **181** (1997) 246.