THE FIVE FIRST VIBRATIONAL STATES OF THE WATER MOLECULE: ROTATIONAL ENERGY AND LINE INTENSITY ANALYSES

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The first part of this paper deals with a global analysis of the rotational levels of water belonging to the (000), (010), (100), (001), and (020) states, for which experimental rotational energies have been obtained using high-temperature flame spectra. The theoretical treatment used is a modified version of the bending-rotation Hamiltonian formalism[a] in which the strong Fermi-type and Coriolis-type interactions occurring in the first triad, already considered[b] in the Watsonian approach, are included. Preliminary analyses show that the theoretical formalism allows us to reproduce the experimental levels up to $J = K_a = 18$ for all five vibrational states. However, a few cases of large Obs.−Calc. differences, which are probably related to interactions between rotational levels of the first triad and those of the second triad are remaining.

The second part of this paper will describe an attempt at determinating the dipole moment function of water through a line intensity analysis. The data set considered consists of transitions belonging to various bands involving vibrational states of the first triad.[c−d] In this second analysis, (an extension in the framework of the large amplitude formalism of the approach[e] initially used for the first triad) line-strengths were determined evaluating the dipole moment matrix elements with the help of the spectroscopic constants obtained in the previous analysis. Work is still in progress, but we hope to be able to compare our results with those obtained through *ab initio* calculations by Jensen *et al.*[f]

[a] L. H. Coudert, *J. Molec. Spectrosc.* **181,** 246 (1997).
[b] J.-M. Flaud and C. Camy-Peyret, *J. Molec. Spectrosc.* **51,** 142 (1974).
[c] R. A. Toth, *J. Opt. Soc. Am. B* **10,** 1526 (1993).
[d] R. A. Toth, *J. Opt. Soc. Am. B* **10,** 2006 (1993).
[e] J.-M. Flaud and C. Camy-Peyret, *J. Molec. Spectrosc.* **55,** 278 (1975).
[f] Per Jensen, S. A. Tashkun, and Vl. G. Tyuterev, *J. Molec. Spectrosc.* **168,** 271 (1994).