H_2O-HF DIMER ROTATIONAL SPECTRA: NEW MEASURMENTS AND RE-ANALYSIS

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New measurements of the H_2O-HF dimer absorption spectrum are performed using a warm (240 - 260 K) equilibrium gas mixture with two complementary spectrometers: a video spectrometer and spectrometer with radio-acoustic detection. We demonstrate that measurements in the millimeter- and submillimeter-wave region allows the rotational spectra of the dimer in its ground vibrational state and in multiple thermally-populated intermolecular vibrational states to be observed. Positions of over hundred H_2O-HF lines in the 158–345 GHz range are refined (their uncertainty is reduced from previous measurments [1] by about order of magnitude) and several tens of lines are newly measured. These data are re-fitted together with previous measurements giving a refined set of constants of effective Hamiltonian which characterizes the dimer intermolecular dynamics. We demonstrate that the new data allow to improve significantly (from 100 to about 10 kHz) the accuracy of rotational constants corresponding to separate series of lines with fixed K_a. Such series-by-series analysis of the spectrum is proposed as a method for identification of lines belonging to thermally populated exited vibrational states of the dimer on the basis of future calculations. Studies of H_2O-HF are important because the system is similar, but easier to study than the important and more complicated water dimer. In particular, unlike the water dimer, H_2O-HF high resolution spectra can be observed and accurately measured at relatively high temperatures.

[1] doi:10.1016/j.jms.2006.11.008, S.P. Belov, V.M. Demkin, N.F. Zobov, E.N. Karyakin, A.F. Krupnov, I.N. Kozin, O.L. Polyansky and M.Yu. Tretyakov, Microwave study of the submillimeter spectrum of the H_2O-HF dimer, J. Mol. Spectrosc. 241, 124-135 (2007).

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