ANALYSIS OF THE ROTATIONAL SPECTRUM OF HDO IN ITS $v_2 = 0$ AND 1 VIBRATIONAL STATES UP TO 2.8 THz

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The rotational and rovibrational spectra of H_2O and its isotopologs, including HDO, are of great importance for atmospheric chemistry, astrophysics, and basic sciences. We recorded rotational spectra of HDO in the ground and first excited bending state from the microwave region up to 2.8 THz. Several spectrometers were employed in Kiel, Köln, and Pasadena. An up-to-date combined analysis with rovibrational data was presented,[a] in which a Hamiltonian based on Euler functions[b] was used to overcome convergence difficulties of the conventional Watson Hamiltonian. The model had been employed previously, e. g., in a related analysis of D_2O spectra with $v_2 \leq 1$.[c] Recently, many more data have been obtained in Köln as well as in Pasadena. Including multiple measurements, these add up to about 230 and 100 new transition frequencies in $v_2 = 0$ and 1, respectively, reaching $J = 17/13$ and $K_a = 9/5$. In addition, a critically evaluated compilation of IR data was published very recently.[d] Difficulties in reproducing the data within experimental uncertainties prompted a reanalysis of the data starting at small quantum numbers and extending the data set in small portions. At lower quantum numbers, difficulties were due to, e. g., few typographical errors and misassignments. At higher quantum numbers, interactions between $v_2 = 0$ and 1 as well as between these and higher states (e. g. $v_2 = 2/v_1 = 1$, which interact through Fermi resonance) are more important. The limitation of the present analysis to the lowest two vibrational states affords some transitions to be excluded from the analysis and causes a truncation of the data set at some values of J and K_a.

[a] S. Brünken, PhD thesis, Universität zu Köln, July 2005, Cuvillier Verlag, Göttingen
[b] H. M. Pickett, J. C. Pearson, C. P. Miller, *J. Mol. Spectrosc.* **233** (2005) 174.
[c] S. Brünken, H. S. P. Müller, C. Endres, F. Lewen, T. Giesen, B. Drouin, J. C. Pearson, H. Mäder, *PCCP* **9** (2007) 2103.
[d] J. Tennyson et al., *J. Quant. Spectrosc. Radiat. Transfer* **111** (2010) 2160.