

Measurements and Analysis of High Resolution Terahertz Spectra of Water

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Abstract.

The advent of future far-infrared and terahertz observatories like SOFIA †, the Herschel Space Observatory or APEX/ALMA ‡ challenges the spectroscopic community to provide accurate transition rest frequencies in this domain to allow for interstellar line identification. Water is the third most abundant molecule in the interstellar medium, and the search for rotational water lines is one of the primary objectives of airborne and satellite-based telescope projects, since its observation from ground-based sites is hampered by its strong atmospheric absorptions. The majority of rotational transitions of H₂O and its deuterated forms HDO and D₂O appear in the Terahertz regime, a frequency domain which is almost completely unexplored by high resolution spectroscopy.

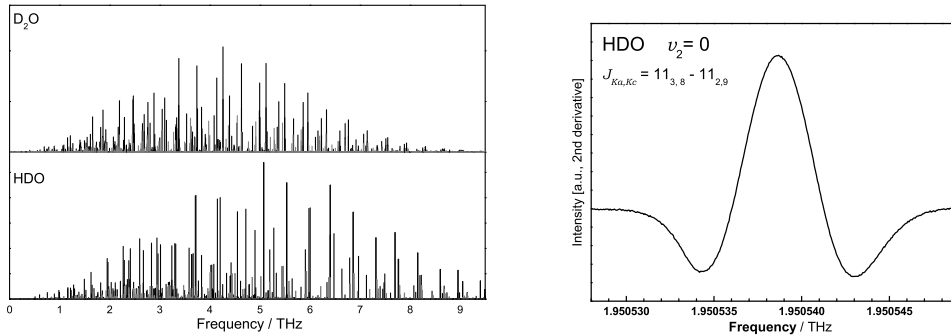


Figure 1. Left: Calculated rotational stick spectra of D₂O (top) and HDO (bottom) in their vibrational ground (black) and first excited bending state (grey) at a temperature of 300 K. **Right:** Exemplary spectrum of a rotational transition of HDO measured with the Cologne Sideband Spectrometer for Terahertz Application in the 2 THz region

We present highly accurate laboratory measurements of the deuterated water species HDO and D₂O in selected frequency regions starting from 8 GHz up to 2.5 THz. Around 280 rotational transitions in both the vibrational ground and first excited bending states ($v_2 = 0, 1$) were measured in total, involving energy levels with to date unexcelled high J and K rotational quantum numbers. The data give valuable information for the spectroscopic analysis of these molecules. In

† Stratospheric Observatory For Infrared Astronomy

‡ Atacama Pathfinder EXperiment / Atacama Large Millimeter Array

the case of the light and non-rigid water molecule, standard methods for its analysis are limited due to large centrifugal distortion interactions. Recently, the so-called Euler expansion of the Hamiltonian was introduced by Pickett *et al.* (2005) for the analysis of these kind of molecules, and its capability was demonstrated for the main isotopomer of water. Here we present a global analysis of rotational and rovibrational data of the $v_2 = 0$ and 1 state of HDO and D₂O by means of the Euler approach. In addition to the newly measured transitions, around 3800 and 2750 lines have been included from previous work for HDO and D₂O, respectively. It was possible to reproduce the extensive dataset to nearly its experimental uncertainty. The improved predictive capability of the model compared to previous work will be demonstrated.

This analysis yields highly precise transition frequency predictions for both species far into the terahertz region which will be made available to the astronomy community *via* the Cologne Database for Molecular Spectroscopy www.cdms.de [Müller *et al.* (2005)].

Keywords. line: identification, molecular data, submillimeter

References

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Müller, H. S. P., Schlöder, F., Stutzki, J., and Winnewisser, G., *J. Mol. Struct.* **742**, 215 (2005).