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NEWS | JULY 03 2020

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Scilight 2020, 271106 (2020)
https://doi.org/10.1063/10.0001493

AIP Publishing

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1 July 2020

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Data enhancement and network-theoretical validation techniques were used to revise a widely utilized 2013 dataset of the rovibrational transitions and empirical energy levels of $H_2{}^{16}O$.

Astrophysics and many other fields require detailed knowledge and accurate understanding of the rotation-vibration spectrum of water isotopologues. The water isotopologue $H_2{}^{16}O$ plays an important role in the Earth's climate as a greenhouse gas in the atmosphere. Furtenbacher et al. assembled the most complete database to date of experimentally measured rovibrational transitions of $H_2{}^{16}O$.

The authors extended an IUPAC database, last updated in 2013, by adding 78 more sources and roughly 100,000 additional entries of transitions, bringing the total number to almost 300,000. The authors also used an improved methodology to shape the collated data. Using network analysis tools they developed, and taking into account updated quantum-chemical results, they were able to identify questionable measurements and inverted the measured transitions to energy levels.

W2020 contains nearly 20,000 rovibrational energy levels with statistically significant uncertainties and a total coverage for the energies of the quantum states of $H_2{}^{16}O$ beyond 9000 cm^{-1}. The 20,000 empirical energy levels represent the measured 300,000 transitions and could facilitate further experiments to yield more energy levels. According to their estimation, the total number of rovibrational energy levels of $H_2{}^{16}O$ is close to one million and most are still unknown.

"Our study defines a new level for water spectroscopy," said author Attila G. Császár. "It is also important to emphasize that the techniques leading to the improved results are general and can be applied to other gas-phase molecules of chemical, physical, and astronomical interest."

Next, the authors are planning to use the same technique to build similar datasets for other water isotopologues, such as $HD^{16}O$ and $H_2{}^{18}O$, which are also atmospheric gases of note.

Source: "W2020: A database of validated rovibrational experimental transitions and empirical energy levels of $H_2{}^{16}O$," by Tibor Furtenbacher, Roland Tóbiás, Jonathan Tennyson, Oleg L. Polyansky, and Attila G. Császár, *Journal of Physical and Chemical Reference Data* (2020). The article can be accessed at https://doi.org/10.1063/5.0008253.