MARVEL analysis of the measured rovibrational spectra of $D_2{}^{16}O$, $D_2{}^{18}O$, and $D_2{}^{17}O$

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This work is aimed toward completing the fourth part of a collaborative effort of an IUPAC Task Group [1,2,3] reporting critically evaluated rotational-vibrational line positions, transition intensities, pressure dependences, and energy levels, with associated critically-reviewed assignments and uncertainties, for all the main isotopologues of water. This work presents validated energy levels and transition data for the following isotopologues of water: $D_2{}^{16}O$, $D_2{}^{17}O$, and $D_2{}^{18}O$.

The latest version of the MARVEL (Measured Active Rotational-Vibrational Energy Levels) line-inversion procedure and code [4] is used to determine the rovibrational energy levels from experimentally measured lines, together with their self-consistent uncertainties. Critical evaluation involves computer-aided handling of a large-scale database of measured transitions assembled from all relevant literature sources. As part of the MARVEL process, a bipartite, two-component spectroscopic network (SN) [5] is constructed from the measured ro-vibrational transitions. The MARVEL process is repeated until self-consistency within the line and level information is achieved. Internal consistency means that the observed transitions can be reproduced, within their stated (and adjusted) uncertainty, not only by the different spectroscopic measurements but also by the MARVEL energy levels.

The lines considered are obtained from spectra recorded in absorption as well as in emission, under widely different physical conditions. During the validation process we check the MARVEL energy levels against the results of sophisticated variational nuclear motion computations. As for $D_2{}^{17}O$ and $D_2{}^{18}O$, further variational computations are performed with the help of the D^2FOPI [6] program in order to check the labels of the experimental transitions via the RRD scheme [7].

The database of $D_2{}^{16}O$ consists of 53 786 measured transitions, connected *via* 11 490 ro-vibrational energy levels. As to $D_2{}^{18}O$, 11 660 transitions were analysed, which yield 3 362 ro-vibrational energy levels. For $D_2{}^{17}O$ only 566 transitions could be analysed, the lines correspond to 338 ro-vibrational energy levels.

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