TOWARDS PERFECT WATER LINE INTENSITIES

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Over the last ten years the increased availability of computational resources and the steady refinement of theoretical methods have permitted more and more accurate first principle calculations of water-vapor spectra as exemplified, e.g., by the very successful BT2 line list[a]. There are two requirements for computing accurate line lists from first principles: a high-accuracy potential energy surface (PES), affecting both line positions and intensities, a reliable dipole moment surface (DMS), affecting line intensities. It is also very useful to several application to give reasonable uncertainty bars for computed quantities, an aspect which traditionally has received little attention. We report here recent progress leading to very accurate room-temperature linelists covering the range 0.05–20 000 cm^{-1}, complete with uncertainty bars, for the $H_2^{18}O$ and $H_2^{17}O$ water isotopologues[b]. Line intensities were produced using a recent DMS produced by our group[c] which is capable of giving line intensites accurate to 1% for most medium and strong transitions. Line positions are based if possible on the experimentally derived energy levels recently produced by a IUPAC task group[d] and have a typical accuracy of 0.0002 cm^{-1}; when experimentally derived energy levels are unavailable calculated line position are provided, with an accuracy of the order of 0.2 cm^{-1}.
An extension to the main isotopologue $H_2^{16}O$ is currently underway.

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