WATER INTENSITIES: AB INITIO VS. EXPERIMENT

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Ab initio calculations of water intensities are becoming mature and are claimed to have 1% accuracy in most cases. Experimental intensities with 1% accuracy can be achieved with some care. An intercomparison ab initio vs. experiment of water intensities for ν_2 ($H_2{}^{16}O$, $H_2{}^{18}O$) and the 1 μm band will be given. Some brief information on the ab initio calculation will be presented while the main focus will be on the experiment and corresponding data analysis. Most of the data show agreement within 2% between ab initio and experiment but part of the data also show larger differences up to 8%. Some of the differences can be attributed to ab initio calculation errors while others originate from experiment. At present experiments are important to validate ab initio but ab initio can be very useful in validating the experiment.