AN ACCURATE POTENTIAL ENERGY SURFACE FOR H_2O

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We have carried out extensive high quality *ab initio* electronic structure calculations of the ground state potential energy surface (PES) and dipole moment function (DMF) for H_2O. A small adjustment is made to the PES to improve the agreement of line positions from theory and experiment. The theoretical line positions are obtained from variational ro-vibrational calculations using the exact kinetic energy operator. For the lines being fitted, the root-mean-square error was reduced from 6.9 to 0.08 cm^{-1}. We were then able to match 30,092 of the 30,117 lines from the HITRAN 96 data base to theoretical lines, and 80% of the line positions differed less than 0.1 cm^{-1}. About 3% of the line positions in the experimental data base appear to be incorrect. Theory predicts the existence of many additional weak lines with intensities above the cut off used in the data base. To obtain results of similar accuracy for HDO, a mass dependent correction to the PES is introduced and is parameterized by simultaneously fitting line positions for HDO and D_2O. The mass dependent PES has good predictive value for T_2O and HTO. Nonadiabatic effects are not explicitly included. Line strengths for vibrational bands summed over rotational levels usually agree well between theory and experiment, but individual line strengths can differ greatly. A high temperature line list containing about 380 million lines has been generated using the present PES and DMF.