AB INITIO CALCULATIONS OF ELECTRIC QUADRUPOLE MOMENT SURFACES AND QUADRUPOLE SPECTRA OF WATER

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The spectrum of water is very important for a broad range of applications including industrial, astrophysical and atmospheric. It is dominated by the electric dipole transitions and is well-studied both experimentally and theoretically, while the much weaker electric quadrupole transitions are less so. Recently we have computed a water line list with the record accuracy of transition frequencies and electric dipole intensities. The high sensitivity of modern spectrometers in terms of absorption coefficients now allow detection of electric quadrupole transitions in absorption through the cavity ring down methods, see the first laboratory detection of an absorption line of the electric quadrupolar band of N₂.

Here we present a new quadrupole line list for 16H₂O generated using a new ab initio electric quadrupole moment surface (QMS) and our empirical potential energy surfaces (PES). The QMS was computed with the CFOUR program suite using the CCSD(T)/aug-cc-pCVQZ level of theory. Intensity calculations were performed using the TROVE and RICHMOL program packages.

The line list will be useful for future detection of electric quadrupole transitions of water as well as for other applications including studies of intermolecular interactions, nonlinear optics, collision-induced spectroscopy and simulation of fluids. The work was supported by the Russian Science Foundation (project 17-19-01602).