PERTURBATIVE CORRECTIONS TO THE CALCULATED TRANSITION FREQUENCY AND OSCILLATOR STRENGTH OF THE HYDROGEN BONDED OH-OSCILLATOR IN THE DONOR WATER MOLECULE IN WATER DIMER

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In order to correct for the inaccuracies of local mode calculated transition frequencies and oscillator strengths of the X-H$\cdots$Y stretch in hydrogen bonded binary complexes, perturbation theory has been applied to the water dimer. In this model the hydrogen bonded OH-oscillator in the donor water unit has been perturbed by coupling to the six low frequency intermolecular modes of the binary complex. The first- and second-order corrections to the energy and the first-order correction to the wavefunction has been obtained for the ground and excited states of water dimer. The method and results obtained using the method on the water dimer will be presented and discussed.