Temperature Dependence Analysis of the NIR Spectra of Liquid Water and QED theory

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Abstract

In this short talk the preliminary results of a very simple experiment could be illustrated. This work has been run in collaboration with Prof. Roumiana Tsenkova, Dr. Zoltan Kovacs and Dr. Antonella De Ninno, and shows some remarkable features of water perturbed by temperature that testify, once more, the bi-phasic nature of liquid water. If looked at by QED theoretical framework hes features can be well explained by first principles, showing that water is not only a stochastic H-bond network. We investigated pure Milli-Q water on increasing the temperature in the vis-NIR range (400-2500 nm). We specifically payed attention to the first overtone region (1300-1600 nm) of the OH-bond stretching-mode where an isosbestic point has been observed. Isosbestic (equal absorption) points are shown when a reaction takes place in a solution where a parameter is changing. Two absorbing components are in equilibrium and, in our experimental set-up, their relative abundance is controlled by the temperature. A second derivative analysis clearly shows two modes, which can be assigned to water molecules involved in different hydrogen bonding. We have also observed that the ratio of these modes follows a van't Hoff behaviour supporting that their energy difference (energy gap) is independent on the temperature. Two phase model of liquid water has been supported recently by several experimental results. We'll show that the two phases differences between energy and entropy estimated from the experimental data can be compared with the prediction of Quantum Electro Dynamics (QED) showing a remarkable agreement.