MICROSOLVATION OF THE GREEN FLUORESCENT PROTEIN CHROMOPHORE ONE WATER MOLECULE AT A TIME

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Solvation plays an important role in the function of fluorescent proteins. Many of these proteins contain a functional water molecule in the chromophore pocket, which can influence the electronic properties of the chromophore. In the case of the Green Fluorescent Protein (GFP), a single water molecule is coordinated to the phenolate group of the chromophore, raising questions about the effect this has on the electronic spectrum of GFP. Here, we present the electronic and infrared spectra of a model system for the GFP chromophore in complexes with up to two water molecules.