STRUCTURAL DEFORMATION OF 4-BENZOYLBENZOATE UPON COMPLEXATION WITH METAL IONS AND SOLVENT UTILIZING MASS-SELECTED CRYOGENIC IR

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4-benzoylbenzoate ($4BBA^-$, $C_{14}H_9O_3$) serves as a model system for the marine organic material in sea-spray aerosols (SSAs), which are highly heterogeneous and complex. SSAs are primarily composed of salt water, which affects the behavior of the marine organic material contained within it. Here, we investigate how addition of metal ions and solvent (H_2O, CH_3CN) modify the structure of $4BBA^-$ by use of cryogenic ion vibrational predissociation spectroscopy. Upon addition of Ca^{2+} to $4BBA^-$, we observe the collapse of the asymmetric and symmetric CO_2 stretching modes due to the bidentate complexation of Ca^{2+} to the carboxylate head group. Upon addition of high dielectric solvent (H_2O or CH_3CN) the vibrational modes are seen to slowly relax towards the vibrational modes of $4BBA^-$. This behavior is explained by electronic structure calculations, showing that the skeletal structure of $4BBA^-$ relaxes towards its original structure with increasing solvation.