INFRARED STUDIES AND TEMPERATURE EFFECTS OF HYDRATED POTASSIUM−CROWN ETHER SYSTEMS

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Ionophores play an important role in the area of molecular recognition because of their ability to selectively bind specific metal ions. In a variety of fields including chemistry and biology, crown ethers are the prototypical model. Two of the most common crown ethers are 12 crown 4 (12c4) and 18 crown 6 (18c6). We have used infrared spectroscopy to study the microsolvation of the $K^+(12c4)(H_2O)_n$ and $K^+(18c6)(H_2O)_n$ systems for n=1-4 in the O−H stretching region of water. Additionally, we will present new studies where these complexes have been tagged with argon. Since the argon-tagged complexes are colder than their untagged counterparts, we can consider the effect of temperature in these systems. These spectroscopic studies, combined with *ab initio* calculations, can be used to characterize the competing non-covalent interactions, and thus understand the molecular basis behind the selectivity exhibited in the condensed phase.