OCTACOORDINATION OF GAS PHASE POTASSIUM IONS

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Recently there has been great interest in understanding the structure and functionality of the KcsA potassium ion channel. The crystal structure obtained by MacKinnon et.al. suggests the coordination of eight oxygen atoms around each of the potassium ions in the KcsA selectivity filter. In bulk water, the coordination number of potassium ions has been reported to be between five and seven. Theoretical studies of hydrated potassium ions have shown a coordination number of eight water molecules only when the waters were restricted from occupying the second solvent shell. The preferred first shell coordination number in the gas phase is determined by a variety of factors, one of the most critical being the magnitude of the ion-ligand interaction. In the case of gas phase potassium ions, the occupation of the second solvent shell occurs for hydration numbers greater than four. By reducing the ion-ligand pairwise interaction, the first shell coordination number may be increased. We have previously used Diflourobenzene (DFB) to reduce the magnitude of the ion-ligand pairwise interaction in a study of the maximum first solvent shell size of gas phase sodium ions. To monitor the stepwise occupation of gas phase potassium ions' first and second solvent shells DFB was added sequentially to $K^+(H_2O)$. Analysis of the IR photodissociation spectra of $K^+(H_2O)(DFB)_{n=4-10}$ in the OH region, shows evidence of the octacoordination of the potassium ion in the gas phase.