SURFACE AND INTERIOR SOLVATED STATES OF METHANOLATED HALIDE CLUSTER IONS

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Hydrated halide ions, with the exception of fluoride, have been found to form surface solvated states, i.e. the ion sits on top of a neutral water cluster. In the case of fluoride, the higher charge density of the ion is able to force the water molecules into an interior solvated state where the ion is at or near the cluster center of mass. In order to better assess the roles of the ion and solvent in the formation of surface states, we have performed experiments on methanolated halide clusters of the form $X^-(CH_3OH)_n$, X = F or Cl. While diprotic water is able to H-bond simultaneously to the ion and another water molecule, monoprotic methanol must choose between forming an ionic hydrogen bond or a hydrogen bond with another methanol. The vibrational spectra of $F^-(CH_3OH)_n$ will be presented and contrasted to the spectra of $Cl^-(CH_3OH)_n$ in the 2.5 to 4 μm range.