

Abstract Submitted
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Solvation of anions by aromatic molecules probed by infrared spectroscopy J. MATHIAS WEBER, HOLGER SCHNEIDER, KRISTEN M. VOGELHUBER, JILA — We have studied the interaction of chloride ions with partially fluorinated benzenes by gas phase infrared photodissociation spectroscopy. Our studies were motivated by the fact that fluorination changes the charge distribution in a benzene molecule. While C_6H_6 has a negatively charged carbon ring and a positively charged hydrogen periphery, C_6F_6 has a positively charged carbon ring and a negatively charged fluorine periphery. If the interaction between a closed-shell anion (such as Cl^-) and the aromatic molecule were based mostly on electrostatic interaction, such an ion would bind to $C_6H_nF_{6-n}$ via the π system for small n and via H bonds to the periphery for large n . We have used IR spectroscopy of Ar solvated $Cl^- \cdot C_6H_nF_{6-n}$ complex anions to investigate if this paradigm holds, using the red shift and intensity increase of CH stretching modes for H-bonded CH oscillators to discern whether Cl^- binds to the π system rather than to the periphery at different levels of F substitution.

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