INFRARED SPECTRA OF CHLORIDE-FLUOROBENZENE COMPLEXES: ELECTROSTATICS VS. H BONDING

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So far, there has been relatively little experimental information on the vibrational spectroscopy of anions involving aromatic molecules. We investigate the behavior of fluorinated benzene molecules as ligands bound to chloride ions. This constitutes a particularly interesting case, as their properties can be subtly tuned through the choice of the number and positions of F atoms in the molecule. The charge distribution in the aromatic ligand changes drastically in going from benzene with its negatively charged ring (π system) and positively charged periphery (H atoms) to perfluorobenzene (positive ring, negative periphery). Consequently, Cl^- binds to C_6H_6 via bifurcated H-bonds in the plane of the ligand, while it binds to C_6F_6 above the aromatic ring. We trace the bonding behavior of $Cl^- \cdot C_6F_nH_{6-n}$ (n = 0 - 5) through the IR spectra of the complexes for all possible numbers and distributions of F atoms.