

An IR and computational study of the pyridine-HCl complex and its fluorinated analogs

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We have been investigating the structural and energetic properties of the 1:1, H-bonded complexes formed from hydrogen chloride (HCl) and pyridine, as well as its fluorine-substituted analogs (e.g., 4-fluoropyridine, 3,5-difluoropyridine, 2,6-difluoropyridine, 3,4,5-trifluoropyridine, and pentafluoropyridine). We have been particularly interested in systems for which the H-bonding and/or partial proton transfer interactions are enhanced by inert, low-dielectric media (solid neon, argon or nitrogen). At this point we are using M06, MP2, B3LYP, ω -B97-XD methods with the aug-cc-pVTZ basis-set to obtain equilibrium gas-phase structures, frequencies, binding energies and charge distributions, which vary systematically with fluorine substitution. However, the key to predicting the condensed-phase effects is to map intermolecular potential along the N-Cl coordinate, both in the gas phase and bulk dielectric media. These profiles vary significantly across this range of complexes. We are also collecting infrared spectra of these complexes in solid neon at 6K, and may also report our preliminary progress on this experimental work.

