A Comparison of Nitrogen-donor-HCl Complexes

C. Soares and J.A. Phillips (mentor)
Department of Chemistry, UW-Eau Claire
Eau Claire, WI 54702

We have been investigating and comparing properties of 1:1 H-bonded complexes between hydrogen chloride (HCl) and pyridine (C_5H_5N), acetonitrile (CH_3CN), formaldimine (CH_2NH), ammonia (NH_3), methylamine (CH_3NH_2) and hydrogen cyanide (HCN). We are particularly interested in systems for which the H-bonding interaction is affected by inert, low-dielectric media (e.g. NH_3-HCl), which can be assessed via matrix-IR experiments. The key to predict the condensed phase effects is to map the intermolecular potential along the N---H and N---Cl coordinates. At this point we are using M06, MP2, B3LYP, wB97XD methods with the aug-cc-pVTZ basis-set to compute potential curves and compare the features of them across this range of complexes, which span a range from strong H-bonds to partial H^+ transfer systems. Recent results from charge analyses, which convey the extent of H^+ transfer, as well as the effect of solvation energies on the N---Cl potential, may also be presented.

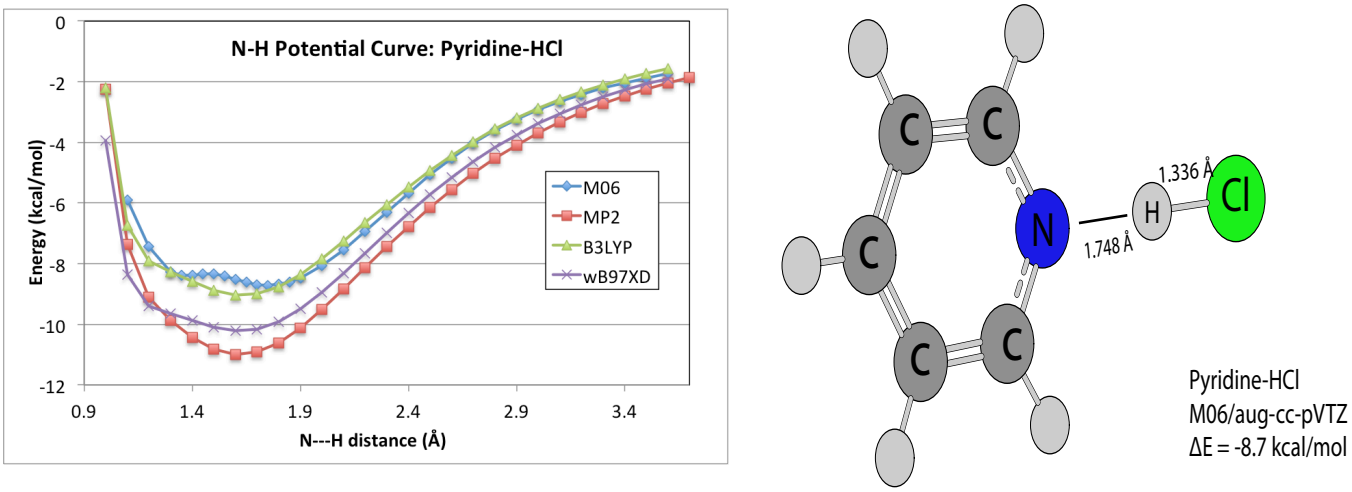

Figure 1: On the left is a potential curve for the N-H distance of the pyridine-HCl complex calculated using four different methods and on the right you see a equilibrium structure of the pyridine-HCl complex.