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PROTON BETWEEN BENZENE AND WATER: INFRARED SPECTROSCOPY TO MODEL INTERACTIONS AT THE OIL-WATER INTERFACE

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The proton affinity of benzene is slightly higher (753.6 kJ/mol) than the proton affinity of water (693.8 kJ/mol) in the isolated gas phase. It is then natural to ask about the location of the proton in the protonated benzene -water complex. Another important question is the effect of solvation on proton accommodation on this system. As benzene is non-polar and water is polar, these kinds of complexes are ideal systems to model molecular interaction at the hydrophobic-hydrophilic interface. In our lab, protonated benzene-water complexes are produced via pulsed discharge in a supersonic expansion cluster source. The cold, mass selected ions are investigated via infrared photodissociation spectroscopy in the range of 1000-4000 cm $^{-1}$. Quantum mechanical calculations were further implemented to obtain the structures and vibrational frequencies. Infrared spectra of the protonated (benzene)$_m$-(water)$_n$ complexes will be discussed, where m=1-2 and n=1-4.