ASSESSING A CLOSE COMPETITION BETWEEN OH-O AND OH-\(\pi\) HYDROGEN BONDING: A HIGH-RESOLUTION IR SPECTROSCOPY OF ANISOLE-METHANOL COMPLEX

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Anisole (C6H5OCH3) has two prominent hydrogen bonding sites, namely oxygen and the \(\pi\)-electrons of the phenyl ring. Earlier studies on anisole-water\(^1,2\) and anisole-methanol\(^3\) complexes show that in both cases the interaction with the oxygen atom is preferred and complex formation takes place via OH-O hydrogen bonding, where water/methanol acts as hydrogen bond donor.

We have studied anisole-methanol complexes in superfluid helium droplets, using high-resolution infrared spectroscopy. Several bands corresponding to (anisole)_m-(methanol)_n complexes (where m=1,2 and n=1) were observed. The size of the clusters corresponding to the observed bands was determined by recording the band intensity as a function of the partial pressures of the constituent molecules, resulting in so-called pickup curves.\(^4\) Based on a comparison of the observed spectra with the predicted spectra, at MP2/6-311++G (d,p) level of theory, we propose that, in helium droplets, for 1:1 anisole-methanol clusters, structures bound via OH-O and OH-\(\pi\) hydrogen bonding are almost equally likely.

References: