A SPECTROSCOPIC STUDY OF CHANGING EQUILIBRIA IN AQUEOUS AND NON-AQUEOUS SULFONIC ACID SOLUTIONS

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Abstract: Sulfonic acids have the general formula RSO$_3$H. They can be found in nature, or synthesised for commercial use in industry as reagents for detergents, dyes, surfactants, sweeteners and drugs. Also, sulfonated resins have been employed as industrial catalysts e.g. in the hydration of propene to iso-propyl alcohol.

In recent years, Raman spectroscopy has advanced from a technique only available in specialist laboratories because of its bulk and the sensitivity of the laser calibration to a technique that is commonly used in and out of laboratories, having been brought into the environment and onto the shop floor.

Further advances have been made in spectral acquisition and now spectra do not take hours but minutes to acquire and as a result “real-time” experimentation has become more common.

In this paper we will discuss the information gathered through “real-time” exploration of saturated solutions of benzene sulfonic acid and p-toluene sulfonic acid in a variety of non-aqueous solvents with addition of metered amounts of water using Raman spectroscopy.

Work has previously been carried out used a Bruker IFS66 FT-IR spectrometer with an FRA106 Raman module emitting at 1064 nm wavelength. Changes in band intensity with gradual shifts in wavenumber were witnessed in the spectra (see Figure 1), however, these spectra were acquired over 30 minutes and the exact time of changes could not be accounted for. Experiments are currently underway using a Renishaw InVia Raman spectrometer emitting at 785 nm wavelength. Quality spectra can be acquired in less than 1 minute and spectral change scan be captured immediately.

Although Raman spectroscopy is insensitive to water, changes in spectra due to hydrogen bonding can still be seen. Zundel et al.\textsuperscript{2} carried out extensive research into hydrogen bonding of polystyrene sulfonic acid using infrared spectroscopy. He found that sulfonic acids are fully dissociated when each –SO$_3$H group is surrounded by two water molecules. Raman spectroscopy should now be able to track the changes in spectra as water is added and hydrogen bonding takes place in the sulfonic acids and evidence of intermediate states of dissociation such as “ionic pairs” or “aggregate clusters” as hypothesised by Edwards et al.\textsuperscript{3} in the case of sulfonated resins may be found.
Figure 1. Benzenesulfonic acid in water

References: