Nuclear Magnetic Resonance Spectroscopy for Measurements of Ion Solvent and Ion Pairing Interactions in Aqueous Solutions

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Ion pairing and ion solvent interactions play an integral role in multiple scientific disciplines such as electrochemistry, biology, geochemistry, and others. In our lab, we are applying nuclear magnetic resonance (NMR) spectroscopy to probe these interactions in aqueous systems. To date we have made measurements for ^{1}H, ^{7}Li, ^{13}C, ^{19}F, ^{23}Na, ^{79}Br, ^{87}Rb, and ^{133}Cs nuclei in simple salt solutions. The NMR spectra resulting from these measurements are simple, typically yielding a single peak, but still require detailed protocols for data collection and analysis. In this talk, we focus on the NMR experiments and discuss the conditions necessary to obtain high-quality, low-uncertainty data for these systems. First, we review the temperature determination method for our measurements and how we account for temperature drifts over time. Next, we examine our frequency referencing scheme that ensures the observed frequency shift of the NMR peaks are accurate and allows for the observation of subtle changes in the NMR peak position as a function of temperature and concentration. Following this, we consider several NMR peak picking methods that were used for choosing the appropriate center frequency for the NMR signal. Finally, we discuss the measurement uncertainty and how it is influenced by both controllable and uncontrollable factors inherent to the systems under investigation.