

## High Pressure Nuclear Magnetic Resonance (NMR) Spectroscopy Experiments to Probe Ion Pairing in Alkali Metal Solutions

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While ion pairing interactions may seem to describe a fundamental chemical process, isolation and analysis of this process remains a significant challenge. Measurement of this particular type of intermolecular interaction requires precise knowledge of the dynamic between solutes, solvents, and the ions of interest. This is particularly useful information for performing chemical separations in the pharmaceutical and biomanufacturing industries. Understanding of ion pairing has largely been informed by a rich abundance of simulation data, but experimental evidence has yet to fully validate these predictions. Most state-of-the-art spectroscopies, such as Raman, infrared, UV, terahertz, small angle x-ray, and neutron scattering, can only probe direct interactions and fail to capture the nuance of ion pairs separated by a solvent shell.

This poster will demonstrate the ways in which high pressure nuclear magnetic resonance (NMR) spectroscopy can be used to further characterize ion pairing behavior utilizing common alkali fluoride salts (NaF, LiF, CsF). By observing trends in the change in frequency of the ion of interest and varying concentration to isolate the paired states, we demonstrate that this well known analytical technique can provide a clearer, more wholistic picture of ion pairing, including solvent effects, and help improve the benchmarks used to simulate such systems.