Exploring Signatures of Ions in Solution with Pair Distribution Function

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Understanding metal ion solvation is central to characterizing and modelling many chemical, biological, and technological processes. However, this phenomenon is complex even for simple salts, involving ion–solvent hydration shells, modified solvent–solvent correlations, and ion–ion interactions.[1] Pair distribution function (PDF) analysis of X-ray total scattering data offers a powerful approach to probe these structural correlations,[2,3] yet the scarcity of systematic experimental data limits the development of generalized models for ion solvation.

Here we present a curated dataset of X-ray total scattering measurements and corresponding PDFs for more than 200 inorganic salts dissolved in water, methanol, and ethanol. The dataset spans a broad range of cations and anions and is provided with consistent processing and detailed metadata. As a case study, we examine chloride solutions across a concentration series to identify distinct solvation patterns and illustrate the structural roles of ions in shaping solution structure.[4] These trends are highlighted in Figure 1, which shows the evolution of the total scattering patterns and corresponding PDFs.

This dataset provides benchmark references for identifying chemical trends in solvation across diverse systems, validating simulations, and interpreting in situ experiments, offering a foundation for improved understanding of solution chemistry and guiding future synthesis strategies.

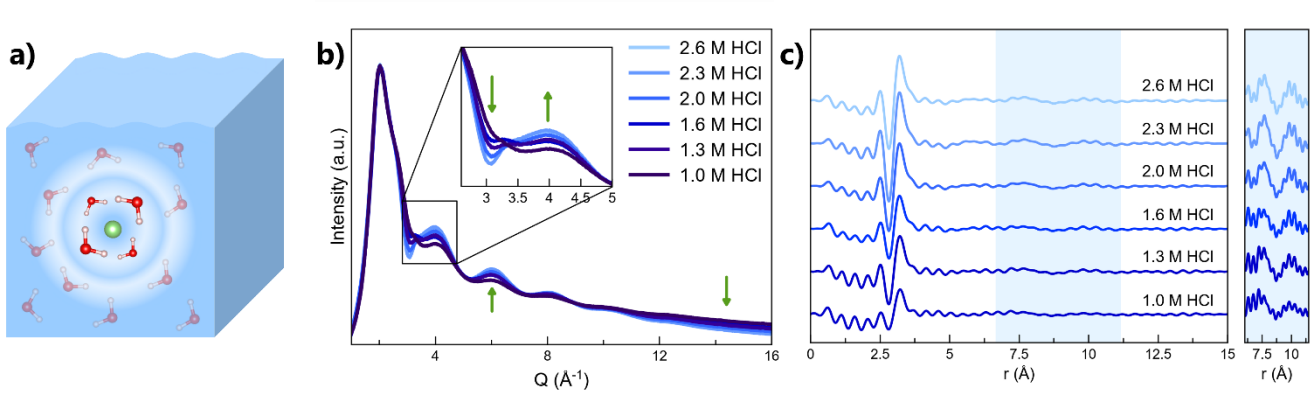


Figure 1. *(a) Schematic representation of the average solvation structure around a chloride ion in water, showing coordination shells of solvent molecules. (b) X-ray total scattering patterns of HCl solutions at varying concentrations, revealing a gradual emergence of structural features at 4 Å and 6 Å. (c) Corresponding Pair Distribution Functions (PDFs), showing increasingly defined features with rising concentration, including indications of longer-range solvation effects at 7.5 Å and 10 Å.*

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