

Neutron diffraction studies of aqueous solutions at elevated temperature and pressure

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Neutron diffraction (ND) provides a powerful means to determine material structure. When combined with the methods of isotopic substitution (NDIS), information can be obtained in terms of interatomic partial pair distribution functions $g_{\alpha\beta}(r)$ and/or as $G_{\alpha}(r)$'s which are linear combinations of these functions associated with an atomic species α .

The NDIS methods are now well-demonstrated in the study of complex liquids [1]. In particular their application to aqueous electrolyte solutions has provided detailed information about all three aspects of the structure, i.e. that of the water solvent, the solute and the ionic hydration. This information has been used to characterise local coordination and ion-water conformations in a variety of systems, and to examine the validity of particular model calculations.

In recent years, the NDIS methods have been extended to include work on solutions under non-ambient conditions, at temperatures up to and beyond the supercritical regime of water. Because neutrons are only weakly scattered by matter, relatively thick pressure containers fabricated from materials such as titanium and its alloys, vanadium, etc. can be used to

obtain neutron diffraction data over a wide range of thermodynamic phase [2].

The talk will contain an up-to-date account of NDIS investigations on water and aqueous electrolytes at temperatures to $\sim 500^{\circ}\text{C}$. It will include results of recent studies of aqueous electrolytes, and describe the changes of ionic hydration and water structure (with temperature and density). A brief account will also be given of similar studies on apolar group hydration, as demonstrated by argon-water mixtures and the commercially important fluid methane in water under pressure. This latter system is particularly useful in probing the fundamental aspects of hydrophobic hydration and the hydrophobic interaction.

References

- [1] Neilson, G.W. and Adya, A.K. (1996) *Royal Society of Chemistry, Annual Reports, Section C*, **93**, 101.
- [2] Neilson, G.W. and Howell, I. (1995) In: *Physical Chemistry of Aqueous Systems* (Eds. H.J. White, J.V. Sengers, D.B. Neumann and J.C. Bellows) 460, Begell House, New York.