Electronic Supplementary Material (ESI) for Faraday Discussions
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A New Structural Technique for Examining Ion-Neutral Association in Aqueous Solution

Supplementary material

Corrections applied to the xylose ICNCI function:

On closer inspection there are clear frequency components in the experimental function with a wavelength of about 4 $Å^{-1}$ that do not occur in the MD function. These are due to molecular correlations and are very clear in the real space representation of this function (Figure 5). If the experiments are performed flawlessly and the multiple scattering and absorption corrections done properly, no such correlations should be visible. However, it should also be born in mind that the final difference function here is a product of four experimental measurements, for each of which the sum of the scattering prefactors is about 400 mb $atom^{-1}$ str^{-1}. The final difference function here is only about 2 mb $atom^{-1}$ str^{-1}. Mathematically the function $\Delta\Delta S^{X}_{H5}(Q)$ is defined as $\Delta S^{X}_{H5}(Q)_{5m}$-1.93 $\Delta S^{X}_{H5}(Q)_{2m}$. However if the subtraction factor is changed from 1.93 to 2.1 (a difference of 9 %), then the comparison is much better. The presence of the molecular correlations (the frequency component with a wavelength of about 4 $Å^{-1}$) is almost entirely removed, as is the gradient due to the Platczek effect. The source of this error is as of yet undetermined. It may be that one of the solutions contained a slightly incorrect atomic concentration, or that the multiple scattering corrections (while being very good), cannot provide corrections to the accuracy such that a difference of 2 mb out of four solutions of 400 mb cannot be predicted within 0.2 mb. However, the comparison with the real space function is still poor. The experimental measurements contain a very large amount of ringing compared to signal. Ideally there should be enough statistical counting over a long enough *Q* range such that no such termination errors occur. However in reality, both the *Q* range and the counting statistic are limited. These factors are highlighted here by the small size of the signal being measured (especially in the important range for this technique, 0-5 $Å^{-1}$, corresponding to the intermediate length scales in g(r) (>~2 Å).

Correction applied to the ICNCI function 2.

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The only correction here was to remove the residual slope. This was performed by fourier filtering (transforming the function into real space, setting it to zero in the *r* range 0-1 $Å^{-1}$, then re-transforming it back into reciprocal space).

No corrections were needed or applied to ICNCI functions 3 and 4.