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The Hybrid technique for accurate transmission XAS on 1-10mM Ni solutions

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XAFS can now be used to investigate electron inelastic mean free paths, dynamical and thermal bonding, to measure nanoroughness and most importantly to assess the significance of alternate hypotheses with derived experimental uncertainty. These key developments will be discussed.

A new approach is introduced for determining XAS spectra on absolute and relative scales using multiple solutions with different concentrations by the characterisation and correction for experimental systematics. This hybrid-technique (HBT) is a development of standard XAFS along the lines of high-accuracy XERT but with applicability to solutions, dilute systems and cold cell environments. We have applied this methodology to determining absolute XAS of [bis(N-n-propyl-salicylaldiminato)] nickel(II) and [bis(N-i-propyl-salicylaldiminato)] nickel(II) complexes with square planar and tetrahedral structures in 15 mM and 1.5 mM dilute solutions. Dilute systems provide excellent XANES and XAFS spectra by transmission, and we confirm that transmission measurements can be superior to conventional fluorescence measurements even for dilute systems. For the first time, we have determined XAS of the isomers from low concentration solutions on an absolute scale with a 1%-5% accuracy, and with relative precision to 0.1% to 0.2% in the active XANES and XAFS regions after inclusion of systematic corrections

[CT Chantler, MT Islam, SP Best, LJ Tantau, CQ Tran, MH Cheah, AT Payne, High accuracy X-ray Absorption Spectra of mM solutions of nickel(II) complexes with multiple solutions using transmission XAS. Journal of Synchrotron Radiation 22 (2015) 1008-1021].

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