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Quality Improvements for Fluorescence Detected XAFS Spectra of Ferrocene

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Methods for the quantification of statistically valid measures of the uncertainties associated with X-ray absorption fine structure (XAFS) data obtained from dilute solutions using fluorescence measurements are developed. Several systematics (e.g. self-absorption) associated in fluorescence detection cannot yet be corrected automatically. Multielement fluorescence detectors provide a set of absolute spectra depending on the geometry of the detector channels with different apparent sensitivities. Error analysis performing the characterization and correction of systematics (self-absorption, energy calibration, photoreduction, air path attenuation etc.) can measure statistical accuracy. Experimental data obtained from 10 mM solutions of the organometallic compound ferrocene, $\text{Fe}(\text{C}_5\text{H}_5)_2$, are analysed within this framework and give robust estimates of the standard errors of the individual measurements. Incorporation of experimental uncertainties into an IFEFFIT-like analysis yield refinement statistics for the staggered and eclipsed forms of ferrocene which show a far more realistic preference for the eclipsed form which accurately reflects the reliability of the analysis. Moreover, the more strongly founded estimates of the refined parameter uncertainties allow more direct comparison with those obtained by other techniques. These XAFS-based estimates of the bond distances have accuracies comparable with those obtained using single-crystal diffraction techniques and are superior in terms of their use in comparisons of experimental and computed structures [CT Chantler, NA Rae, MT Islam, SP Best, J Yeo, LF Smale, J Hester, N Mohammadi, F Wang, Stereochemical analysis of Ferrocene and the uncertainty of fluorescence XAFS data, *J Synch. Rad.* 19 (2012) 145-158].

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