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To merge or not to merge; to spline or ...

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Common preprocessing and published spectra in XAFS, EXAFS and XANES destroys much of the information content of the data, and limits any possible reanalysis, verification or independent further inquiry. There are several key causes for this, which we discuss here. While the raw data from a synchrotron or laboratory experiment is necessarily incomplete and can normally not stand on its own, in principle it has inherent measures of stability, precision and a range of information on accuracy and inconsistencies. Hence this raw data could be extremely useful if the content was somehow explained and preserved. Advanced XAFS experimental methods such as the X-ray Extended Range Technique, the Hybrid technique, and others have explicitly intended to capture and preserve the key contributions to these limitations. Further, while the presentation of processed chi vs energy or k^2 chi vs k plots, or transformed chi vs r plots are common in the thousands of publications per annum, even the processing from [mu/rho] for absorption measurements or the fluorescence measured ratios for fluorescence measurements lose a lot of information and information quality in the common application of a defined E_0, and background removal, and spline fitting of the atomic reswponse abocve the edge, and the removal of the spline function and the presentation of chi vs E or k. We explain the dangers here and the value of raw data (or non-processed data) in this respect.
Most quality data involves either n repeat scans where n is from 3-10, typically; or in fluorescence very often 36 or 100 pixels in a fluorescent detector pixel array. However, many software analysis programs compute a simple or blind average without computing or reporting a precision or self-consistency measure, and the information content for hypothesis testing is lost. We explain part of the physics required to preserve this information and therefore the need either for raw data or carefully and minimally preprocessed data to preserve the key scientific value and information content for hypothesis testing. Accordingly, we present plots of both [mu/rho] v E and chi or k^2 chi vs k for most data sets, but we also provide [mu/rho] v E, error analysis on both axes, i.e. raw preprocessed files with background information, as deposited material for [all] datasets. In part because of the approach, we find that this can enable a sensitivity to structure and model which did not exist with processed data.

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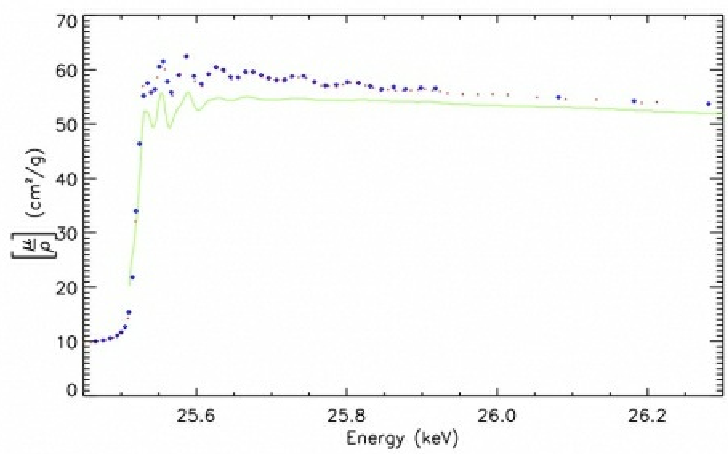

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