INTERNATIONAL TABLES FOR CRYSTALLOGRAPHY

ISSN 1574-8707
it.iucr.org

Volume I, X-ray Absorption Spectroscopy and Related Techniques
ISBN: 978-1-119-43394-1

Chapter 3.43

The X-ray extended-range technique for higher accuracy measurements and higher significance of X-ray absorption spectroscopy results

Christopher T. Chantler*

School of Physics, University of Melbourne, Parkville, Victoria 3010, Australia. *Correspondence e-mail: chantler@unimelb.edu.au

Keywords: X-ray absorption spectroscopy; X-ray fluorescence; X-ray extended-range technique; XERT; systematic errors; accuracy; uncertainty.

The X-ray extended-range technique (XERT) is an advanced high-accuracy technique for X-ray attenuation, X-ray absorption spectroscopy (XAS), X-ray absorption fine structure, X-ray absorption near-edge structure and fluorescence XAS which has been developed and applied at several beamlines around the world. The statistical precision and accuracy of data obtained using XERT, compared with standard experiments using the same beamline and flux, are normally improved by a factor of 10–100. Of course, it takes a longer period of data collection in order to return greater physical and chemical insight. XERT has successfully been applied across the energy range from 5 to 60 keV. It has been applied to elemental materials from silicon ($Z = 6$) to tin and gold ($Z = 79$) and it has been applied to K edges and L edges. It has successfully been applied to monoelemental metal foils, solid compounds, crystals and concentrated (15 mM) and dilute (1.5 mM) solutions, and to systems with from 100%(w/w) to 0.07%(w/w) of the active species in the molecule of interest. XERT has measured attenuation and absorption coefficients from 4 to 340 g cm^{-2} with samples of thicknesses from 1 µm to 4 mm and natural logarithm ratios $0.01 < \ln(I_0/I) < 9$. XERT has been applied to transmission measurements and fluorescence measurements, and to active-species attenuations as low as $\ln(I_0/I) = 0.001$ for solutions. The principles, techniques and technology of XERT should directly carry across to soft X-ray, *in vacuo* and vacuum ultraviolet energies. Whereas standard XAS may attain a precision or accuracy as low as ~1–10%, XERT has regularly reached a precision and accuracy of 0.1% or 0.02%, depending upon the material, beamline and energy regime. Simpler approaches have many valid purposes, but the higher accuracy of XERT permits several novel opportunities: (i) investigations of nanostructure and local structure, and not just 'fingerprinting', (ii) determination of nanostructure against multiple hypotheses, and not just 'confirmation of structure from some other technique', and (iii) *ab initio* structural determination that is equal to, or in some cases better than, that from X-ray diffraction for local structure (Glover & Chantler, 2007). This accuracy permits the observation of dynamic structure, and the evolution thereof, compared with the anisotropic thermal parameters and ellipsoids obtained from X-ray or neutron diffraction. For many fundamental questions, it is a key tool for future research.

Related chapters

Volume I: 3.7, 3.11, 3.12, 3.13, 3.14, 3.37, 3.38, 3.39, 3.42, 3.44, 3.45, 3.46

Many beamline experiments have gone beyond the earlier practice for X-ray absorption spectroscopy (XAS) of measuring once and quickly to obtain a result to confirm a key structure or active site. Many have used multiple repeated measurements as a marker for beam damage, monochromator lagging, heat-load settling, robustness and heterogeneity of a sample over space or time, or simply the determination of variance and precision based upon the uniformity and consistency of measurements (see Chantler, 2024*a*). Numerous expert investigators and groups, or beamline staff, have probed one specific, perhaps dominant, systematic error in their sample or data set. Optimization in general for an

https://doi.org/10.1107/S1574870723009485

XAS experiment depends critically upon the sample, the energy and the question to be addressed, upon whether the experiment is in transmission or fluorescence mode, and upon the region of interest, whether X-ray absorption fine structure (XAFS), pre-edge, X-ray absorption near-edge structure (XANES), extended XAFS (EXAFS) or all of the above.

The X-ray extended-range technique (XERT) followed the studies on the stability of attenuation measurements carried out as part of the International Union of Crystallography (IUCr) X-ray Attenuation Project (Mika *et al.*, 1985; Creagh & Hubbell, 1987, 1990; Creagh, 1987). This originated in part because surveys of attenuation or absorption coefficients reported in the literature often found discrepancies from one another of 10–30%, including across edges.

XERT commenced with the view (Chantler *et al.*, 1999) that investigating as many unknown systematic errors across an extended range of energies, sample morphologies, beam footprints and attenuations will work towards the attainment of the greatest accuracy and insight for reference data sets, for cross-platform investigations and for data sets for deposition for XAS, XAFS and XANES. XERT has particularly been developed by Chantler, Barnea, Tran, de Jonge and a series of students and collaborators since 1999.

Since 2010, several publications have emphasized the need to consider four key contributions to systematic and structural errors in XAS and XAFS measurements (Harmonics, Alignment, Linearity and Offsets; ‘HALO’; Bunker, 2010). Efforts to control, measure and correct for dark current, dead time and energy calibration were called for in the conclusion of the summary of the original Q2XAFS meeting (Ascone *et al.*, 2012). Abe *et al.* (2018) emphasized the need for the control of noise, variance, dead time, dark current, detector nonlinearities, harmonics, uncompensated Bragg glitches and self-absorption. The general topic of calibration and diagnostics is introduced in Diaz-Moreno (2024).

In this first work (Chantler *et al.*, 1999), the principles of XERT drew upon the conclusions of the IUCr X-ray Attenuation Project, listing ten areas of inquiry and systematic errors in typical experimental measurements of attenuation or XAS that should be investigated and addressed (Chantler, 2009).

(i) At least 25% of prior measurements ‘may have had significant contamination from higher harmonics’ (Creagh & Hubbell, 1987). This affects background, edge jumps and attenuation and absorption coefficients, potentially with an energy-dependent structure. Hence, harmonics should be characterized and preferably monitored and measured (Barnea & Mohyla, 1974).

(ii) Some 33% of the surveyed results ‘made no correction for dead time, dark current or detector nonlinearities’. This changes the structure, especially near-edge oscillations and amplitudes, and prevents transmission measurement detectors from responding linearly. In fluorescence, this may be dominated by effects in the upstream detector (dark current) or in the fluorescence detector (dead time). Hence, dark current and dead time should be characterized, monitored and measured.

(iii) Some 33% of the surveyed results used (usually laboratory) configurations with a large divergence. For transmission, this broadens and lowers the downstream signal and dampens the XANES oscillations, and makes an effectively thicker and wedge-like sample. For fluorescence measurements, this broadens the range of fluorescence absorption in the sample and the range of incident and take-off angles. Hence, divergence should be controlled, as is quite normal for transmission synchrotron measurements.

(iv) For single crystals or oriented samples, Bragg–Laue diffraction should be avoided by rotation around the azimuthal angle and by collimation, or it should be monitored and characterized. In general, the nature of the sample should be evaluated carefully before measurement.

(v) The ‘Nordfors criterion’ relates to an optimal attenuation ratio for accurate measurement, $2 < \ln(I_0/I) < 4$ (Nordfors, 1960; Creagh & Hubbell, 1987), based upon two perfect detectors in transmission. In XAS measurements, this is normally chosen or matched above the edge. Therefore, with a single sample it is usually not possible for the sample to match the criterion below the edge of interest. This criterion also does not allow for noise, background signal, detector nonlinearities, flux and key systematic errors, and thus needs to be better explored and characterized. In part, this argues for at least one optimal thickness above the edge and at least a second optimal thickness below the edge; in general, it argues for the use of several sample thicknesses to characterize the full XAS region. In particular, interpretation of measurement statistics and precision is critical. More generally, the criterion following the optimization of the statistic yields a value for $0.2 < \ln(I_0/I) < 8$ under normal conditions (Chantler, Tran, Paterson, Cookson *et al.*, 2001), especially with multiple samples.

(vi) Scattering contributions are related to these issues and are usually unmonitored and undiagnosed. The nature of elastic scattering , whether Bragg–Laue, Rayleigh or thermal diffuse scattering, is critical. Each of these has different angular dependencies. Inelastic (Compton) scattering will usually be directed as a dipole towards 90° from the incident beam. Fluorescence radiation emitted by the atomic scatterer is isotropic in nature but is shaped by the orientation of the sample and the detector to provide angular dependence at small forward and backward angles, and its contribution is often very important. In general, some attempt should be made to measure and investigate the dominant scattering or fluorescence in the experiment.

(vii) For poor samples (for example carbon and nanostructures), small-angle scattering can arise from voids and defects, with errors in the apparent or nominal thickness or integrated column density and impact upon the signals in the detectors. Alternatively, perhaps, a full-foil mapping can be used to monitor sources of sample structure or heterogeneity in the beam.

(viii) Most results do not characterize the thickness of the sample in the X-ray beam (the integrated column density).

(ix) Few results have a characterized statistical precision.

(x) The monochromation, *i.e.* resolution and bandwidth, may be inadequate to resolve additional structure. The beam-on-sample bandwidth often dampens the XANES and white-line amplitudes and structure, and can distort the experimental definition of the edge energy.

These issues remain of concern today. In addressing these issues, we have undertaken measurements across large ranges of energy and attenuation (XERT); repeated these 3–10 times for each point and each sample [to determine the variance and precision, as raised in (ix) above]; with low divergence, (iii); repeated across several sample thicknesses for suitable samples (to investigate detector linearity and scattering orientational dependence), (iv), (v) and (vi); repeated across several aperture combinations (to investigate fluorescence and scattering contributions); with direct repeated measurements of dark current (to investigate detector linearity), (ii), and of a blank (to investigate detector efficiency and to isolate tthe sample from the environment); and taken harmonic measurements using daisy wheels (to measure harmonic contamination), (i); with periodic measurements of energy (not just one point measurement at the edge); and with characterization of the sample average mass and thickness and a full-foil mapping, (vii) and (viii). In general, we have looked for and found the impact of bandwidth in the beam, and hence we have measured and extracted this from the data, (x).

Using this approach, we were able to observe and measure harmonic contamination, even down to 10^{-5}, from its effect upon daisy-wheel or calibrated sample measurements (Chantler, 2024*b*, 2024*c*), observe thermal diffuse scattering behaviour (Chantler, Tran, Paterson, Barnea *et al.*, 2001; Sier *et al.*, 2020), Rayleigh scattering behaviour (Chantler, Tran, Barnea *et al.*, 2001), Bragg–Laue scattering behaviour (Tran, Chantler *et al.*, 2003; Chantler, 2009) and fluorescence, where they were significant in an experiment, from anomalies between samples or orientation or from aperture measurements in a daisy wheel (Sier *et al.*, 2022; Chantler, 2024*b*), observe nanoroughness of a sample by comparison with other (smooth, thicker) samples (Glover *et al.*, 2009; Chantler, 2024*b*) and recalibrate powder diffraction standards for lattice spacing and use these to determine absolute energies to a fraction of an electronvolt in the central X-ray energy ranges (Chantler *et al.*, 2004, 2007; Rae *et al.*, 2006).

Following Tran, Barnea *et al.* (2003*a*) and de Jonge *et al.* (2004), the absolute calibration for the sample thickness in the beam on sample consists of the following.

(i) Obtaining the average thickness of the thickest specimen(s) by weighing it and carefully determining its area.

(ii) Mapping the thickness of the specimen using a micrometer.

(iii) Mapping the relative thickness (that is, the integrated column density) of the central part of the specimen(s) using X-rays.

(iv) Combining the results of the above three measurements and hence determining the average thickness of the ‘1 × 1 mm’ area from the defining upstream collimating slits with divergence, through which the collimated X-ray beam actually passes during the attenuation measurement.

(v) Relating the thicknesses of all other specimens to the absolute thickness of the thickest specimen by measuring their relative absorption of X-rays at one or more energies.

For equivalent studies of solutions, the concentration and cell depth are usually less well defined, but can be normalized by a blank including the empty cell and by using multiple concentrations. Usually, these solution cells cannot be mapped *per se*; yet they can be referenced to an additional reference sample which has been mapped.

Here, we provide a general summary of principles, following Chantler *et al.* (2010).

(i) We do not assume that the monochromator axis is highly calibrated under arbitrary or adaptive step sizes (in step scans or continuous or slew scans) of energy, nor do we use a single relatively beam-dependent calibration foil edge to determine the energy based upon a tabulation of reference energies and an inflection point. We have shown that these assumptions may have an energy-dependent error across an extended absorption edge of several electronvolts or even up to 100 eV (Chantler *et al.*, 2004; Tran *et al.*, 2004; de Jonge *et al.*, 2007). Instead, we independently calibrate the monochromated, delivered energy using either powder diffraction standards (silicon or LaB_6) or single-crystal standards (silicon or germanium), depending upon the beamline, which maps out the energy axis for the measurements involved and removes the slope error and higher-order hysteresis. Some 10–12 points of energy are usually used to calibrate the energy and the encoder offsets, but even two or three points measured in this manner can avoid several systematic errors. An edge energy or E_0 error of only 6 eV in measurement or refinement analysis (for example using an XAFS code) can yield a 3.2% error in lattice spacing, radial bond distances and overall scale (Glover & Chantler, 2007).

(ii) The step size in energy should be commensurate with the absorption structure. A finer grid is used near edges. This part of our technique has developed over several experiments since the earlier experiments focused on accurate individual attenuation or absorption measurements rather than near-edge structure, XANES and XAFS. Other expert XAFS groups have used advanced macros for this for many years.

(iii) For each energy, we measure multiple samples with a range of thicknesses and attenuation ratios, or multiple solution concentrations of the active species or solute. We use multiple samples, addressing alignment uncertainty and impurity contamination by testing the sample dependence of attenuation and random error. Seven to 15 samples of varying thickness cover the range. For each energy, a minimum of three sample thicknesses quantify scattering, detector and sample systematic errors (thickness, linearity and alignment errors). These sample thicknesses are generally chosen to investigate a wide range of attenuations to quantify these systematic errors. Our multiple-foil technique calibrates detector-response nonlinearities.

(iv) For each sample, we measure several different aperture combinations to the upstream and downstream detectors using daisy wheels (Chantler, 2024*b*). This serves to characterize any backscattering or forward-scattering components from the beam and therefore to obtain an accurate total attenuation measurement. By characterizing the scattering and fluorescence contributions, we can also help to determine the separated photoabsorption coefficient from the total attenuation coefficient.

(v) For each sample–aperture combination, we measure the dark current (the noise level of the detector chain), the blank (air measurement without the sample, an empty solution cell or a solvent with no solute) and the sample. This normalizes the signal to a baseline and calibrates for air or path attenuation and scattering.

(vi) For each combination, we typically repeat the measurement ten times to provide a robust estimate of random or correlated noise and hence precision or time-dependent drifts. The raw repeatability of a measurement is usually limited by synchrotron beam fluctuations, but the precision of the normalized signal is often below 0.01%.

(vii) Periodic tests are made for harmonic contamination of the beam using a series of daisy wheels mounted on either side of the samples (Chantler, 2024*b*, 2024*c*). Our daisy-wheel and wedge devices measure harmonic contributions and enable high-accuracy calibrations of detector performance. At extreme energies or on insertion devices, large harmonic contamination is difficult to isolate. An undiagnosed 0.1% contamination by a higher harmonic can invalidate an experiment, especially for edge-jump and background measurements or measurements of the absolute absorption coefficient.

(ix) Detailed materials characterization is performed to map the measured values to a calibrated absolute attenuation coefficient. This includes measurement of thickness profiles and impurity tests, and mapping of the average mass per unit area of the samples.

Our analysis typically follows the logic below.

(i) Calibrate the measured energy points and establish the functional offset and curvature of the hysteresis of monochromator readings. Search for any energy drifts or motor or crystal relaxation effects during the measurements.

(ii) Normalize the count rates for air and beam optic absorption and scatter, and for detector base noise. Optimize the detectors, apertures and geometry for high correlation between upstream (normalizing monitor) and downstream (detector) ion chambers, and hence determine point precision and consistency.

(iii) Use the material or standard characterization to determine the absolute thickness of the sample region in the X-ray beam. Check the alignment of the material and optimize the angle so that it is perpendicular to the beam (for purely transmission measurements; for fluorescence measurements we normally align at 45° to the beam with the detector at 90° to the beam). Transfer this thickness calibration to all other foils to give absolute accuracies with error bars.

(iv) Use daisy wheels to independently check for harmonic contamination and correct where necessary. Confirm by comparison with absorption by a foil or sample.

(v) Compare the different aperture measurements using the daisy wheels and search for the effects of scattering. Correct the raw total attenuation coefficient for any scattering effects observed.

(vi) Compare the different thicknesses and search for the effects of bandwidth and roughness. Search for the signature of any remaining unexplained systematic errors.

(vii) Propagate the errors and summarize the results.

The XERT approach was extended (Chantler *et al.*, 2015; Islam *et al.*, 2016) to the study of millimolar solutions in transmission mode and also in simultaneous transmission and fluorescence mode. This led to the development of the hybrid technique, especially because using multiple thicknesses was not usually possible in a single solution cell, so the definitions of blank and thickness were generalized to include the blank (empty) cell, the blank cell (with solvent but no solute or active species), even if in a cryostat, and a series of concentrations across a range where, for example, the local structure is assumed to be unchanged. This also led to adapted techniques for cryostat use, *i.e.* low temperatures and temperature series where, for example, it is not normally possible to make a 'sample mapping' or 'full-foil mapping'. These measurements can still be normalized using a reference foil or sample in transmission, typically outside and downstream of the cryostat and measured sequentially. Some differences are required in preparation for fluorescence measurements and in processing the data (Chantler, 2024*d*).

The definition of a hybrid technique is a little variable or vague because it adapts to the experimental conditions and constraints and is usually significantly faster than simplifying XERT for some particular systematic errors. Indeed, many expert users have implemented key components of XERT and hence can be regarded as using advanced, high-accuracy or hybrid techniques. This is perhaps exemplified by John *et al.* (2023) and this very important grey area in terminology is explained and summarized in Best & Chantler (2024*d*).

A brief summary of some typical key diagnostic results is presented following Ekanayake *et al.* (2021*b*) in Table 1. The relative uncertainty of XAFS accuracy or structure can be below 0.001%, and the absolute measurement of attenuation can be accurate to below 0.023%. Some individual contributions can be addressed by choosing an ideal foil thickness, by characterizing the foil particularly well before measurement, by choosing a thin foil, especially with respect to the Nordfors criterion, by choosing a thick foil, especially with respect to the Nordfors criterion, or by explicitly measuring the dark current and the blank as recommended within XERT, but most of the corrections invoke multiple foils and multiple repetitions of measurements to obtain the reported accuracy and precision.

Table 1 presents the uncertainties and variation of mass attenuation coefficients for zinc metal foils at the Australian Synchrotron and the magnitude of specific systematic corrections. The contributions to measurements are labelled $[\mu/\rho]_{\rm rel}$ if they particularly contribute to the relative structure of adjacent points, the edge shape or the XAFS, or $[\mu/\rho]_{\rm abs}$ if

Table 1
Uncertainty and variation of mass attenuation coefficients for zinc metal foils at the Australian Synchrotron at 8.5–11.59 keV using XERT (Ekanayake *et al.*, 2021*b*).

Quantity	Magnitude of correction $[\mu/\rho]$	Uncertainty and variance $\sigma_{[\mu/\rho]}$	Comments
$[\mu/\rho]_{\rm rel}$		<0.319%	Variance[a]
	22–536% (10 μm foil)	<1.853% (10 μm)	Blank normalization[b]
	Up to 97% (50 μm foil)	<0.133% (100 μm)	
	Up to 57% ± 15% (100 μm)	0.00039–1.46%	Dark current[c]
	Up to 1.31% (10 μm)		
(total)		<0.042%	Total variance after corrections[d]
	1–5 × 10^{-3}%		Harmonic correction[e]
(50 μm)	<14.2%	<10.5%	Fluorescence correction[f]
(25 μm)	<0.101%	<0.003%	
(10 μm)	<0.0123%	<0.0003%	
(total)	<0.139%	<0.028%	
(10 μm)	<2.52%	<0.02%	Roughness[g]
(25 μm)	<0.815%	<0.015%	
(total)	<1.56%	<0.0037%	
(50 μm)	<9.89%	<0.239%	Bandwidth[h]
(25 μm)	<4.91%	<0.119%	
(10 μm)	<1.703%	<0.041%	
(total)	<7.24%	<0.0037%	
$[\mu/\rho]_{\rm abs}$		<0.037%	Nominal thicknesses[i]
	3.55–7.60%	0.000018–0.024237%	Average ICD[j]
	0.374–7.606%	0.024%	Full-foil map[k]
E (keV)	−1 to +3 eV ± 1–3 eV	<0.0038%	Energy[l]

Quantity	Magnitude range ($\rm cm^2\,g^{-1}$)	Uncertainty range $\sigma_{[\mu/\rho]}$	Comments
$[\mu/\rho]_{\rm rel}$	34.765–325.321	0.000677–0.027%	After systematic corrections[m]
$[\mu/\rho]_{\rm abs}$	34.765–327.760	0.023–0.0357%	After normalizing to absolute thickness from full-foil map[n]

[a] Standard errors from counting statistics (variance including precision before systematic corrections). [b] Blank correction and net uncertainty (Section 3 in Ekanayake *et al.*, 2021*a*). Large for thin foils. [c] Dark-current correction and net uncertainty (±0.5 counts $\rm s^{-1}$; Section 3 in Ekanayake *et al.*, 2021*a*). [d] Total dispersion of measurement precision after the above corrections. [e] Harmonic coefficient and contribution is very small here (Section 7 in Ekanayake *et al.*, 2021*a*). [f] Secondary photons from fluorescent scattering. The correction is large for the 50 μm sample and directly above absorption edges and is zero below the Zn edge (Section 6 in Ekanayake *et al.*, 2021*a*). Maximum uncertainty only applies to the 50 μm sample. [g] The effect of roughness is greatest for the 10 μm sample when the attenuation is large (Section 8 in Ekanayake *et al.*, 2021*a*). [h] The bandwidth correction is greatest for the 50 μm sample along the edge where $d[\mu/\rho]/dE$ is greatest. [i] Use of nominal thickness and the corresponding uncertainty (Sections 4 and 5 in Ekanayake *et al.*, 2021*a*). [j] Use of local integrated column density and the corresponding uncertainty (Section 5 in Ekanayake *et al.*, 2021*a*). [k] Absolute accuracy of the full-foil mapping technique (Section 4 in Ekanayake *et al.*, 2021*a*). [l] Error in the energy calibration data. The correction is minimal at the absorption edge (Section 9 in Ekanayake *et al.*, 2021*a*). [m] Relative measurements and uncertainties after correcting for systematic errors. [n] Absolute measurements and uncertainties after normalizing to absolute thickness with a full-foil map.

they primarily scale all values with a slowly varying function. Hence, there are two final uncertainties relating to the absolute value of the mass attenuation coefficient $[\mu/\rho]$ and relating to the pointwise and local structure, for example for XAFS analysis, which can be denoted $[\mu/\rho]_{\rm abs}$. Some magnitudes of systematic error correction are very large for thicker samples, as convention might suggest, such as dark current, whilst some are much larger for what might have been thought of as ideal thicknesses, such as for blank normalization and roughness. Some are strongly structural across the XAFS region, while others are predominantly localized to a region of the XAFS, for example the near-edge or XANES regions. Others are smooth corrections across the whole XAS and thus may not affect the detailed XAFS structure but may affect the magnitudes of the oscillations and hence the fitted parameters of S_0^2 as normally processed. This table is an illustration of key systematic errors for this particular experiment and beamline; however, numerous other systematic errors have been observed and diagnosed in other experiments on other beamlines using XERT, including monochromator drift, Bragg reflections from the sample and harmonics.

In conclusion, the need for multiple repetitions of XAS measurements, typically up to ten, to provide a variance and precision in transmission or fluorescence is recognized in general and is highly recommended for all studies including XANES and pre-edge studies. In general, the need to measure and monitor the dark current (upstream and transmission) and the dead time (fluorescence) remains important and is possible for all studies. Some blank measurement (without foil, without solute or without solvent for an empty cell) is important for all studies and can be accommodated in routine work with relatively little effort. The use of daisy wheels or some equivalent measurement or monitor of harmonics and fluorescence is often important near the edges.

Sayers (2000*b*) recommended

> Harmonics passing the X-ray monochromator should be evaluated *quantitatively*, and the methodology used to eliminate them should be reported. If possible a harmonic detector should be operated throughout the data collection.

Also, they recommended that

> If possible, representative samples should be measured at two different thicknesses. This is a good overall test for a range of thickness related effects, including sample non-uniformity, harmonic content of the beam, and leakage . . .

and

> Many of the issues raised . . . require equipment in addition to the two ion chamber absorption setup. Instead of each group supplying such equipment, it makes more sense for the facility to provide it.

Further, Sayers (2000*a*) recommends, as a general principle,

> Reports of all quantitative results that are derived from XAS measurements must be accompanied by an estimate of the uncertainty and a description or a citation that explains the basis for that uncertainty.

References

Abe, H., Aquilanti, G., Boada, R., Bunker, B., Glatzel, P., Nachtegaal, M. & Pascarelli, S. (2018). *J. Synchrotron Rad.* **25**, 972–980.

Ascone, I., Asakura, K., George, G. N. & Wakatsuki, S. (2012). *J. Synchrotron Rad.* **19**, 849–850.

Barnea, Z. & Mohyla, J. (1974). *J. Appl. Cryst.* **7**, 298–299.

Best, S. P. & Chantler, C. T. (2024). *Int. Tables Crystallogr. I*, ch. 3.14, 375–394.

Bunker, G. (2010). *Introduction to XAFS: A Practical Guide to X-ray Absorption Fine Structure Spectroscopy.* Cambridge University Press.

Chantler, C. T. (2009). *Eur. Phys. J. Spec. Top.* **169**, 147–153.

Chantler, C. T. (2024*a*). *Int. Tables Crystallogr. I*, ch. 4.6, 617–623.

Chantler, C. T. (2024*b*). *Int. Tables Crystallogr. I*, ch. 3.39, 539–543.

Chantler, C. T. (2024*c*). *Int. Tables Crystallogr. I*, ch. 3.38, 537–538.

Chantler, C. T. (2024*d*). *Int. Tables Crystallogr. I*, ch. 2.8, 88–99.

Chantler, C. T., Barnea, Z., Tran, C. Q., Tiller, J. B. & Paterson, D. (1999). *Opt. Quantum Electron.* **31**, 495–505.

Chantler, C. T., Islam, M. T., Best, S. P., Tantau, L. J., Tran, C. Q., Cheah, M. H. & Payne, A. T. (2015). *J. Synchrotron Rad.* **22**, 1008–1021.

Chantler, C. T., Rae, N. A. & Tran, C. Q. (2007). *J. Appl. Cryst.* **40**, 232–240.

Chantler, C. T., Tran, C. Q. & Barnea, Z. (2010). *J. Appl. Cryst.* **43**, 64–69.

Chantler, C. T., Tran, C. Q., Barnea, Z., Paterson, D., Cookson, D. J. & Balaic, D. X. (2001). *Phys. Rev. A*, **64**, 062506.

Chantler, C. T., Tran, C. Q. & Cookson, D. J. (2004). *Phys. Rev. A*, **69**, 042101.

Chantler, C. T., Tran, C. Q., Paterson, D., Barnea, Z. & Cookson, D. J. (2001). *Radiat. Phys. Chem.* **61**, 347–350.

Chantler, C. T., Tran, C. Q., Paterson, D., Cookson, D. & Barnea, Z. (2001). *Phys. Lett. A*, **286**, 338–346.

Creagh, D. C. (1987). *Nucl. Instrum. Methods Phys. Res. A*, **255**, 1–16.

Creagh, D. C. & Hubbell, J. H. (1987). *Acta Cryst.* A**43**, 102–112.

Creagh, D. C. & Hubbell, J. H. (1990). *Acta Cryst.* A**46**, 402–408.

de Jonge, M. D., Barnea, Z., Tran, C. Q. & Chantler, C. T. (2004). *Phys. Rev. A*, **69**, 022717.

de Jonge, M. D., Tran, C. Q., Chantler, C. T., Barnea, Z., Dhal, B. B., Paterson, D., Kanter, E. P., Southworth, S. H., Young, L., Beno, M. A., Linton, J. A. & Jennings, G. (2007). *Phys. Rev. A*, **75**, 032702.

Diaz-Moreno, S. (2024). *Int. Tables Crystallogr. I*, ch. 3.48, 581–585.

Ekanayake, R. S. K., Chantler, C. T., Sier, D., Schalken, M. J., Illig, A. J., de Jonge, M. D., Johannessen, B., Kappen, P. & Tran, C. Q. (2021*a*). *J. Synchrotron Rad.* **28**, 1476–1491.

Ekanayake, R. S. K., Chantler, C. T., Sier, D., Schalken, M. J., Illig, A. J., de Jonge, M. D., Johannessen, B., Kappen, P. & Tran, C. Q. (2021*b*). *J. Synchrotron Rad.* **28**, 1492–1503.

Glover, J. L. & Chantler, C. T. (2007). *Meas. Sci. Technol.* **18**, 2916–2920.

Glover, J. L., Chantler, C. T. & de Jonge, M. D. (2009). *Phys. Lett. A*, **373**, 1177–1180.

Islam, M. T., Best, S. P., Bourke, J. D., Tantau, L. J., Tran, C. Q., Wang, F. & Chantler, C. T. (2016). *J. Phys. Chem. C*, **120**, 9399–9418.

John, M. W., Sier, D., Ekanayake, R. S. K., Schalken, M. J., Tran, C. Q., Johannessen, B., de Jonge, M. D., Kappen, P. & Chantler, C. T. (2023). *J. Synchrotron Rad.* **30**, 147–168.

Mika, J. F., Martin, L. J. & Barnea, Z. (1985). *J. Phys. C Solid State Phys.* **18**, 5215–5223.

Nordfors, B. (1960). *Ark. Fys.* **18**, 37–47.

Rae, N. A., Chantler, C. T., Tran, C. Q. & Barnea, Z. (2006). *Radiat. Phys. Chem.* **75**, 2063–2066.

Sayers, D. E. (2000*a*). *Error Reporting Recommendations: A Report of the Standards and Criteria Committee.* http://ixs.iit.edu/subcommittee_reports/sc/err-Rep.pdf.

Sayers, D. E. (2000*b*). *Report of the International XAFS Society Standards and Criteria Committee.* http://ixs.iit.edu/subcommittee_reports/sc/.

Sier, D., Cousland, G. P., Trevorah, R. M., Ekanayake, R. S. K., Tran, C. Q., Hester, J. R. & Chantler, C. T. (2020). *J. Synchrotron Rad.* **27**, 1262–1277.

Sier, D., Ekanayake, R. S. K. & Chantler, C. T. (2022). *X-ray Spectrom.* **51**, 91–100.

Tran, C. Q., Barnea, Z., de Jonge, M. D., Dhal, B. B., Paterson, D., Cookson, D. J. & Chantler, C. T. (2003). *X-ray Spectrom.* **32**, 69–74.

Tran, C. Q., Chantler, C. T., Barnea, Z., Paterson, D. & Cookson, D. J. (2003). *Phys. Rev. A*, **67**, 042716.

Tran, C. Q., de Jonge, M. D., Barnea, Z. & Chantler, C. T. (2004). *J. Phys. B At. Mol. Opt. Phys.* **37**, 3163–3176.