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

Validation procedures for XAFS

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Suggested validation checks for XAFS data sets are tabulated together with the datafile contents necessary to carry out these checks.

Keywords: validation procedures.

1. Introduction

Well defined machine-readable metadata allow the automatic validation of internal data-set consistency and are a useful tool for both developing and promoting community standards for data presentation. For example, *CheckCIF* (Strickland *et al.*, 2006) includes an extensive set of data-validation routines applied to datafiles written according to the CIF standards, and is widely used by structure-publishing journals to assess the quality of the experiment upon which a crystal structure is based; with the advent of agreed XAFS metadata definitions and file formats, similar levels of validation would be possible for XAFS data.

2. Required metadata

A shared and well defined collection of data names allows journals, peak XAFS bodies and XAFS databases to specify data names that should be included in a datafile in order to

Table 1
Example validation checks for an XAFS datafile.

Data-processing stage	Validation check	Required data names (in general may take multiple values)
Raw data	Do the reported data correspond to the specified experimental setup? Are ionization detector counts provided for all detectors? If fluorescence detector counts are included, has the detector been described? Are any data channels missing?	Detector type, detector position, number of fluorescence detector channels, measured detector signal
Data reduction	Have the absorption values been correctly derived from the observed counts (including error propagation)? Is the stated sample composition and thickness approximately consistent with the observed absorption? Does the absorption edge occur in the correct region? Have multiple channels been correctly merged? Have monitor counts been correctly applied? Have out-of-range detector readings been appropriately handled? Has wavelength been correctly converted to energy?	Energy, wavelength, monochromation type, monochromator parameters, absorption, sample thickness, sample phase composition, measured sample density, absorption edge name
Data fitting	Does subtraction of the stated background functions reproduce the provided XAFS curves? Does the stated atomic model reproduce the fit? Are the fitting statistics correct? Is the atomic model chemically reasonable?	Calculated and experimental XAFS, k value, coefficients in equation for pre-edge background, spline coefficients, atomic positions, occupancies and displacement parameters, k-weighting scheme, Fourier filter settings, source of theoretical XAFS calculations

meet a particular standard. Initial validation then checks for the presence of these data names. A further level of validation examines data-name values to ensure that they are both within acceptable ranges and self-consistent. Table 1 lists some possible XAFS datafile consistency checks, together with generic data names that must be included in the file in order to carry out the checks. Note that many data names for describing crystal structures have already been defined within the Crystallographic Information Framework and need not be redefined for XAFS work.

References

Strickland, P., Hoyland, M. A. & McMahon, B. (2006). *International Tables for Crystallography*, Vol. G, edited by S. R. Hall & B. McMahon, pp. 561–562. Dordrecht: Springer.