MAX (Multiplatform Applications for XAFS) New Features

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Abstract. MAX is a complete suite of XAFS data analysis computer programs, written with the cross-platform object scripting language Livecode [1] working on Windows, MacOSX and Linux systems, freely available on our web site since 2007 [2]. The 2009 version presentation is available in the XAFS14 conference proceedings [3] and regularly updated on the www.xafs.org web site [4].

1. Introduction

MAX is composed of 5 modules (figure 1):

1) Absorbix, 2) Cherokee, 3) Crystalffrev, 4) Roundmidnight (divided in RoundMidnightRev, RoundMidnightFit and RoundFitAuto), which will be described in detail only for their original functions, new features and improvements included since XAFS14 conference.

5) Straight no Chaser, which is totally new and deserves to be described in more details.

2. Modules description

2.1. Absorbix

Absorbix is a utility for sample absorbance calculations. It can calculate and optimize total absorbance and edge jump of pure samples, mixtures of solid powdered sample with solid solvents (recently improved), and liquid solutions. It includes also fluorescence self-absorption corrections, for EXAFS and for XANES.
2.2. Cherokee
Cherokee includes raw data conversion to absorption curves (with various input data files formats), predge and atomic absorption baselines removal, XANES and EXAFS normalization, Fourier Transform and Filtering, experimental EXAFS data statistical error estimation. The main new feature of this program is the Multiple Data modules, which add to the standard single spectrum data treatment, the possibility to open, calculate and display quickly spectra issued from multiple data files. This is especially useful for time-resolved experiments with many data files to treat in almost automatic sequences.

2.3. Crystalffrev
Like Bruce Ravel’s ATOMS included in ARTHEMIS code [5], CRYSTALFFREV is a crystallographic tool for the conversion of crystal structures clusters centered on absorbing atoms, in order to created FEFF input files.

The main differences are:

a) FEFF7 and FEFF 8 entries (FEFF9 available soon)

b) Import/Export file formats. In addition to a specific Crystalffrev input/output file format, CIF and PDB import/export file formats are also available.

c) Crystal Space group search. A more complete compilation of the most recent version of the IUCr International Tables of Crystallography space groups, with a space groups synonym dictionary and search tools for alternate definitions, and non-conventional crystallographic symmetry operations editing.

d) Cluster rotation. The possibility to rotate the local cluster axis in order to choose the orientation of the z axis (very useful for axial ligand analysis of macrocycle metalloenzyme active sites).

e) Crystal disorder tools. Partial substitution and vacancies random distribution generator for multiple partial occupancy sites in disordered materials.

New: A normally distributed random atomic position generator in order to simulate translational disorder and random radial distribution function of selected atoms in the cluster.

In development:

1) FDMNES [6] input files editing.

2) Non gaussian RDF generator for disordered crystal structures.

2.4. Roundmidnight
Roundmidnight is our EXAFS fitting program, composed of 3 modules: RoundMidnightRev, RoundMidnightFit and RoundFitAuto. The fit of theory versus experimental EXAFS is based on the standard multiple scattering and spherical waves EXAFS formula as documented in FEFF ab initio code, and the general function minimization software MINUIT from the CERN computer library [6].

Roundmidnight is totally compatible with FEFF, both in the fitting module, and in the multiple scattering paths analysis module. However, any other sources of phase and amplitude functions are also admitted. The empirical mean free path curve can be fitted on model standards and used in place to, or in combination with, the FEFF reduction factor and calculated photoelectron mean free path in order to improve the EXAFS fit in the low k (<3Å⁻¹) domain.

The fitting procedure follows the IXS Standard and Criteria error subcommittee definitions and recommendations [7] on statistical error estimation (both students statistics on several exafs recordings and fourier noise filtering methods), reduced Δc² (quality factor QF, calculated either in k or R spaces), parameter correlations and fitting convergence criteria. In addition, we have implemented a F-test calculator [8]. A “batch” module is available, in order to edit, run and analyze the results of multiple fits of input files.

In the previous versions RoundmidnightRev was only able to prepare input files for the fitting routine RoundmidnightFit (which was opened by hand by the user) and analyse the result. The most
important new feature since 2009 is the possibility to run automatic fits directly from the main program RoundMidnightRev in one button click, since the new Roundfitauto external routine is launched and run automatically. RoundMidnightRev contains also a FEFF scattering paths analysis module.

2.5. Straight no Chaser.
This new member of the MAX family is a linear algebra fit program in order to decompose mixed spectra in their model components. The linear decomposition of mixed xafs spectra on the basis of a priori known model spectra was developed first.

The program provides fitted molar or mass ratio (if the user provides the model compounds molar mass), and their standard error bars. It works on normalized XANES, complete normalized absorption or EXAFS spectra.

Linear Least Squares Fit is performed by Gauss-Jordan matrix inversion or by Single Value Decomposition (SVD, preferable). It provides statistical Quality Factor (QF), error bars and correlation matrix, tools to check and minimize the correlations and improve the fit accuracy, when possible.

Designed to treat multiple set of spectra, Straight no Chaser can quickly open multiple model compounds and sample spectra in a few clicks.

We propose two special features:
1) A Progressive Linear Least Squares method in order to find the best composition using three constrains: i) fitted coefficients must be positive, ii) errors on the fitted coefficients must be less than x% of the values, x set by the user, iii) when both i and ii criteria are fulfilled, choose the composition with the lowest QF. This procedure was found to be very useful when the actual number of components among the possible model compounds spectra is unknown and some of the model spectra are highly correlated.

2) Fit automatically a series of N spectra (N only limited by the computer memory, and the computing time). This module can be used to fit automatically series of spectra issued from a Quick EXAFS experiment and plot the composition evolution versus time or any physical parameter.

When the *a priori* knowledge of the model compounds in the unknown samples is incomplete, other linear algebra statistical tools, based on SVD, must be available: Principal Component Analysis and Target Transformation [9] modules are under development and will be available soon in Straight no Chaser.

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