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FASTOSH: a software to process XAFS data for geochemical & environmental applications

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FASTOSH is a standalone program to process X-ray Absorption Fine Structure (XAFS) spectroscopy data collected at SAMBA, Synchrotron SOLEIL, or any other XAFS beamlines generating data files in ascii format. Imported functions from Larch [1] allow normalizing XAFS spectra and conveniently background subtracting EXAFS scans collected with a step-by-step or rapid continuous acquisition mode. The main graphical interface is user-friendly and inspired from Athena featured in Demeter & Ifeffit Software Package [2]. The code, written in Matlab 2016b, enables beam line users to follow in real-time the progress of their acquisition. It also proposes an interactive background-subtraction tool for Multi-Channel Analyser (MCA) patterns. This can help minimize, in the XAFS spectrum extracted from MCA patterns, distortions due to acquisition artefacts such as diffraction phenomenon arising from well-crystalline solid or frozen liquid samples. Additionally, the code features auto deglitching options, and a PCA/Target Transformation module that can instantaneously process a large library of XAFS spectra. It also proposes a tool to post-treat data processed by the MCR-ALS Matlab Toolbox of Jaumot et al [3]. Consequently, this program should be particularly useful for geochemical and environmental applications where the XAFS technique is employed.

[1] Newville M. (1995) *J. of Physics : Conf. Series* 430, conf. 1. [2] Ravel B. & M. Newville, (2005) *J. of Synchr. Rad.*12, 537–541. [3] Jaumot *et al.* (2005) *Chem. & Int. Lab. Systems.* 76, 101–110