FOX (Free Objects for Xtallography)

FOX (Free Objects for Xtallography) is a free, open-source program for windows and Linux written for ab-initio structure determination from powder diffraction (SDPD). It performs direct-space structure determination using the reversed Monte Carlo algorithm of global optimization, allowing a modular description of the structure as a combination of atoms, polyhedra and molecules. Since the first release of FOX in 2001 [1], many features have been added in order to enhance all steps required for a successful SDPD, along with various useful tools to explore crystal structures and powder diffraction patterns [2-7].

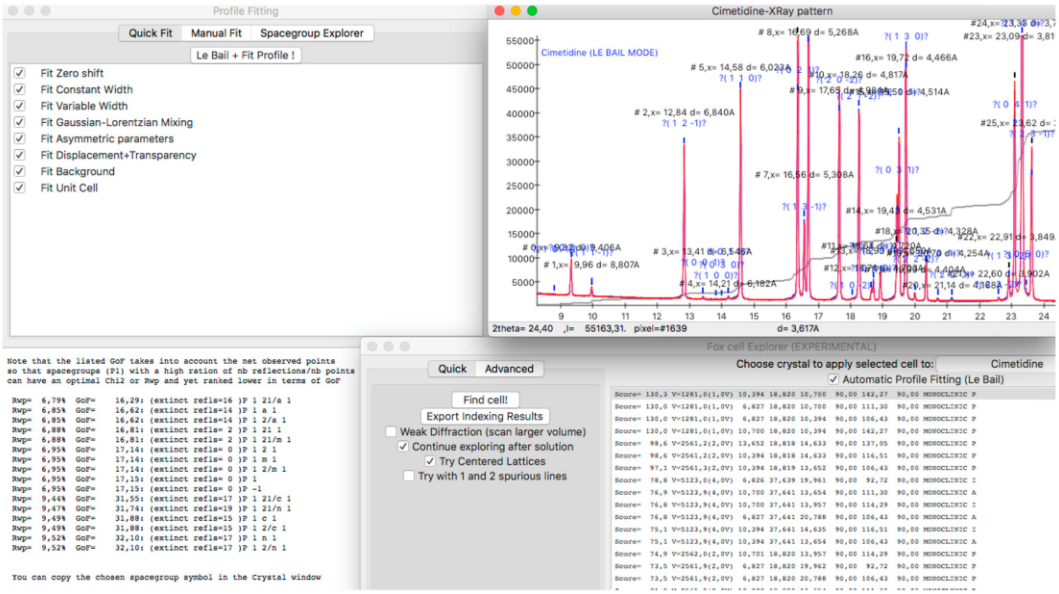

Figure 1. FOX 2017.2 indexing and profile fitting interface. **Top left**: profile fitting widget, allowing to select groups of parameters to optimize using Le Bail and full-profile least squares. **Bottom left**: result of the space group explorer, where all space groups compatible with the unit cell are tested and listed with increasing Goodness-of-Fit. The correct choice in this case is the first one, with the highest number of systematic extinctions. **Top right**: zoomed portion of the observed and calculated powder pattern in profile fitting (Le Bail) mode, with the list of peaks found and predicted indexing. **Bottom right**: results from a 'quick' indexing, with solutions listed by decreasing M_{20} score.

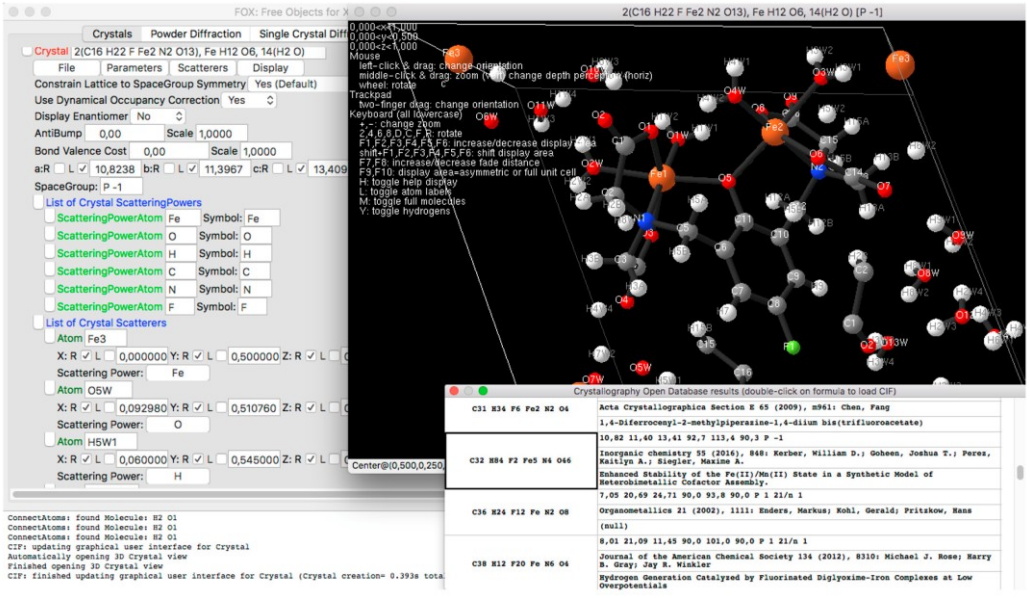

Figure 2. Main FOX interface. Left: main window with the beginning of the description of a crystal structure. Top right: 3D view of the structure, with the help text, showing only the asymmetric unit. Several shortcuts are available to easily toggle between different views (full unit cell, toggle hydrogens, fade atoms outside display volume…). Bottom right: result of querying the Crystallography Open Database [8], after searching for structures with elements C, N, O, F, Fe and 6 different elements. A simple double-click allows to load the CIF in FOX, where the molecules are automatically built by analysing the atomic distances.

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