

CrysFML: a Library to Develop Crystallographic Programs in Fortran 95. Powder diffraction examples

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CrysFML is a set of Fortran 95 modules to be *used* in crystallographic and diffraction computing programs [1]. Modern array syntax and new features of Fortran 95 are used through the modules. We take advantage of all object oriented programming techniques already available in Fortran (user-defined types, encapsulation, overload of procedures and functions). The lacking features (e.g. inheritance and class methods) will be easily implemented as soon as compilers of the new standard become available. We aim to preserve the efficiency, the simplicity and the adequacy of modern Fortran for numerical calculations. All aspects of symmetry and handling of reflections and structure factor calculations are treated in dedicated modules. Main programs using the adequate modules may perform more or less complicated calculations with only few lines of code. The documentation is written in the source code. A document, in HTML format can be generated using a program.

We shall present a an overview of the present status of the library and a series of examples useful for powder diffraction: simple crystallographic calculations, bond-valence sums, aids to space group determination, profile fitting, powder diffraction simulations, kernel of the Rietveld method, etc.

[1] Rodríguez-Carvajal J., González-Platas J., *Compcomm Newsletter* 2003, **1**, 50.

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