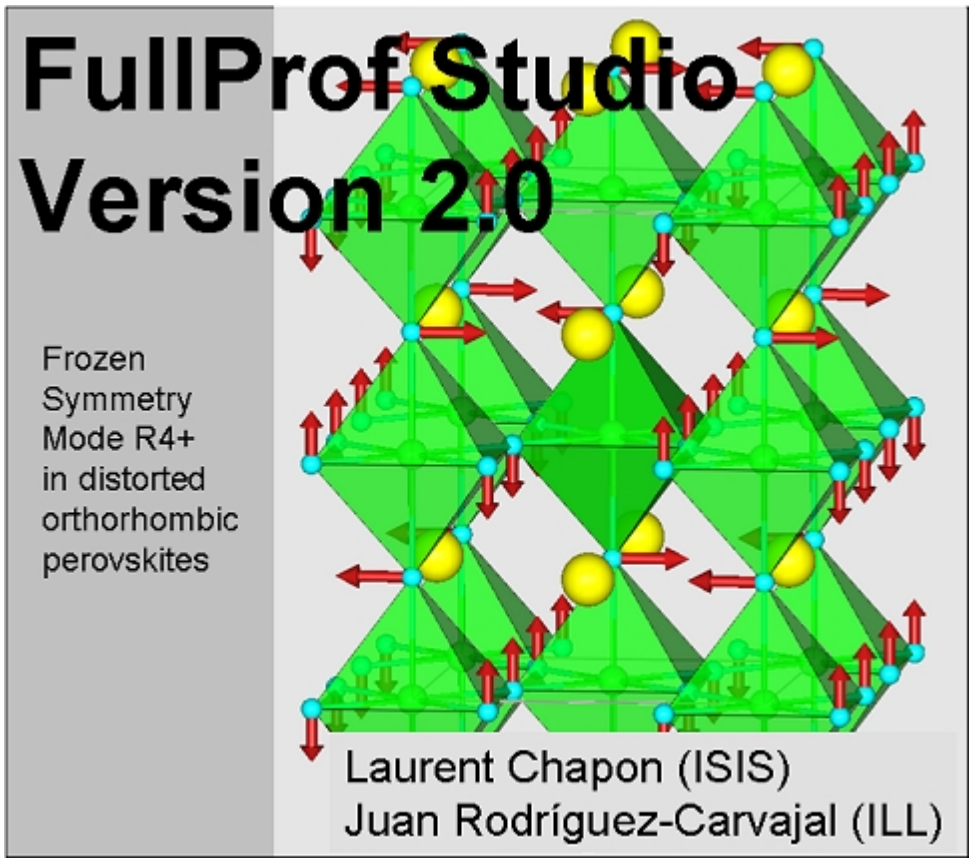
FpStudio

Welcome



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Introduction

The version 2.0 of the FullProf Studio (***FpStudio***) program is being distributed with the current version of the FullProf Suite. The program ***FpStudio*** has been developed for visualising crystal and magnetic structures. The program has been written by Laurent Chapon (ISIS, RAL) and it is based in the ***WCrysFGL*** (Laurent Chapon & Juan Rodríguez-Carvajal) and ***CrysFML*** (Juan Rodríguez-Carvajal & Javier González-Platas) Fortran 95 crystallographic libraries. This is the result of an informal collaboration between ILL (Grenoble, France) and ISIS (Didcot, UK) in data treatment with the aim of providing useful tools for free to the scientific community using diffraction techniques for structural research.

The program uses the Winteracter library (Interactive Software Services Ltd.) and OpenGL.

Running the program

A present the program runs on Windows and Linux/MacOS platforms. Here we describe the use of ***FpStudio*** in a Windows platform but it is easily to translate to Linux/MacOS versions.

- The program can be run from a DOS shell typing **fp_studio**, clicking on its icon or from the ***FpStudio*** button in Toobar of the FullProf Suite  .
  The program can also be invoked with an argument corresponding to the input file as:

```
My_prompt> fp_studio codfefiln <cr>
```

- The program can automatically be invoked from ***WinPLOTR*** if the keyword "draw_fst" (without quotes) is written in the appropriate place in the "winplotr.set" file. This is, for instance, what you have to introduce in "winplotr.set":

```
[AFTER FULLPROF RUN]
 plot_prf no_edit_pcr draw_fst
```

The input file for ***FpStudio*** has the extension ".fst" (called hereafter FST file) and it is automatically generated by ***FullProf*** after a structure refinement. So after running FullProf with "codfefil.pcr", as input file, the program generates the files "codfefil*n*.fst" (where *n* stands for the number of the phase).

The interface is intuitive enough so that a normal Windows user can immediately explore what FullProf Studio can perform.

Input File

All lines starting with"!" are considered as comments.

Structure Directives

For plotting a crystal structure the following keywords are needed:

- ATOM
- BKG
- BOND
- BOX
- CELL
- CONN
- POLY
- SPACEG

ATOM

ATOM *Label ChemSymb x y z [plot options]*

This keyword give the atom information.

The additional options are given for plotting purposes. At present they are:

- DISPLAY (default)
- NODISPLAY
- RADIUS
- COLOR

Example:

ATOM Cu1 CU 0.0 0.0 0.5 RADIUS 0.8 COLOR 0.8 0.8 0.1 1

BKG

BKG *color_value*

It controls the background colour.

To instruct ***FullProf*** to generate an FST file with this keyword, the corresponding instruction to be given in the PCR file, has to be put in the line with the name of the phase.

BOND

BOND *Label1 Label2 dist_min dist_max [plot options]*

The ***dist_min*** and ***dist_max*** represens the distance range between the two given atoms for creating a bond between them.
Additional plotting keywords may be added in the same line. There is no limit for the number of BOND keywords.

The additional options are given for plotting purposes. At present they are:

- DISPLAY (default)
- NODISPLAY
- RADIUS

- COLOR

Examples:

BOND Cu1 Cu1 0 3.3 RADIUS 1.0 COLOR 1 0 1 1

BOND Cu1 O1 0 2.4 RADIUS 0.2 COLOR 0 1 1 1 NODISPLAY

BOX

BOX *xmin xmax ymin ymax zmin zmax*

Represent the volume of the structure to be considered for plot

Example:

BOX -0.15 1.15 -0.15 1.15 -1.25 1.25

CELL

CELL *a b c* α β γ

Define the cell parameters

Example:

CELL 4.32 4.32 8.41 90.0 90.0 90.0

CONN

CONN *ChemSymb1 ChemSymb2 dist_min dist_max [plot options]*

This keyword is similar to BOND but the atom names correspond to atomic species instead of atom labels. Bonds are generated between all atomic species separated by a distance within the given interval.

Example:

CONN Cu O 0 2.4 RADIUS 1.0 COLOR 0 1 1 1

GENER

GENER *symmetry*

Instead of giving the space group a list of generators is also admissible. The keyword is then GENER followed by the symmetry operator given in symbolic form. Up to 15 generators are allowed.

Example:

GENER x,-y,z+1/2.

POLY

POLY *LABEL [COLOR RGBA] [EDGES] [RADIUS x.x] [EDGECOL RGB]*

LABEL		Particular atom or chemical species in the list
COLOR	RGB	Red-Green-Blue codes. Real numbers between 0 and 1.
	A	Transparency control. A=0.0 corresponds to a completely transparent (invisible) object and A=1.0 to an opaque one.

EDGES		Means that the edges of the polyhedra will be emphasized.
RADIUS	XX	Edges will be drawn using the given radius, by default the radius is 1.
EDGECOL	RGB	Colour of the edges (by default is black 000).

This keyword allows the generation of polyhedra around central atoms.

To be operational previous BOND or CONN directives have to be given in order to make the program calculate the surrounding atoms.

Examples:

```
POLY Cu2
POLY Ni3 color 1 1 0 0.5
POLY Fe1 color 0.6 0 0 0.5 EDGES
POLY Cu2 color 1 0 0 0.6 EDGES EDGECOL 0 0 1
POLY Fe1 color 0.6 0 0 0.5 EDGES
```

SPACEG

SPACEG *Spacegroup*

Spacegroup is the string containing the Hermann-Mauguin symbol of the space group given in the same format as in ***FullProf***

Example:

SPACEG I 41/a m d

Magnetic Directives

For plotting magnetic structures, we need in addition the definition of the propagation vector, magnetic symmetry and Fourier coefficients of the magnetic moments. For starting the magnetic part description a brace "{" must appears in the first column. The magnetic description bloc finishes with a line containing a closing brace, "}", in the first column. In the current version only a single magnetic block per file is allowed but several propagation vectors can be grouped into a single magnetic block. The Fourier components are given in a separate line from `MATOM`. Depending of the way the user describes the magnetic structure, in the case of several propagation vectors, the produced FST file may have to be changed manually in order to represent the real structure.

The content of the magnetic part is the following:

- ARROW_DISP
- K
- LATTICE
- MATOM
- MSYM
- SKP
- SYMM

ARROW_DISP

ARROW_DISP

This keyword may appear outside the braces defining the magnetic structure.

This makes the position of the arrow starting from the centre of the atoms. This is quite convenient for describing displacement vectors of symmetry modes.

K

K *Pv1 Pv2 Pv3*

Components of the propagation vector with respect to the reciprocal basis of the conventional unit cell.
Several **K** keywords can appear in a single magnetic block.

Example:

K 0.500 0.000 0.123

LATTICE

LATTICE *Symbol*

This keyword is, normally, the lattice symbol of the Space group.

Example:

LATTICE I

MATOM

MATOM *Label ChemSymb x y z [plot options]*

This is similar to ATOM keyword. There's no limit for the number of **MATOM** lines.

The additional options are given for plotting purposes. At present they are:

SCALE *value*	Re-scale the magnetic moments
GROUP	Fourier coefficients corresponding to different propagation vectors have to be grouped to calculate the total magnetic moment.
ENVELOP *attributes*	For case of a single propagation vector (**k**,-**k**) and an atom having imaginary components on the Fourier coefficients. The keyword and attributes adopt the form: ENVELOP *ENVELOPCOL 0 1 0 0.50 EDGE EDGECOL 1 0 0 1 RADIUS 2.00*

MSYM

A block of symmetry operators similar to that appearing in the PCR file for a magnetic phase when Isym=-1.

SKP

SKP *n1 n2 Rx Ry Rz Ix Iy Iz MPhas [Optional keywords]*

n1	Number of the propagation vector in the block
n2	Number of magnetic matrices to be applied (see FullProf manual)
Rx *Ry* *Rz*	$\mathbf{S}_{\mathbf{k}} = \frac{1}{2}\{\mathbf{R} + i\mathbf{I}\}\exp(-2\pi i\,\phi)$
Ix *Iy* *Iz*	$\mathbf{S}_{\mathbf{k}} = \frac{1}{2}\{(R_x, R_y, R_z) + i(I_x, I_y, I_z)\}\exp(-2\pi i\,MPhas)$
MPhas	

The Fourier coefficients of the magnetic structure are written just following the MATOM lines.

When **k** is not equivalent to -**k** (so both terms $\mathbf{S_k}$ and $\mathbf{S_k}^*$ are included in the sum). If **k** is equivalent to -**k** (a single term) then $\mathbf{S_k}$ =**M**= (R_x, R_y, R_z) and **I**=0, *MPhas*=0

SYMM

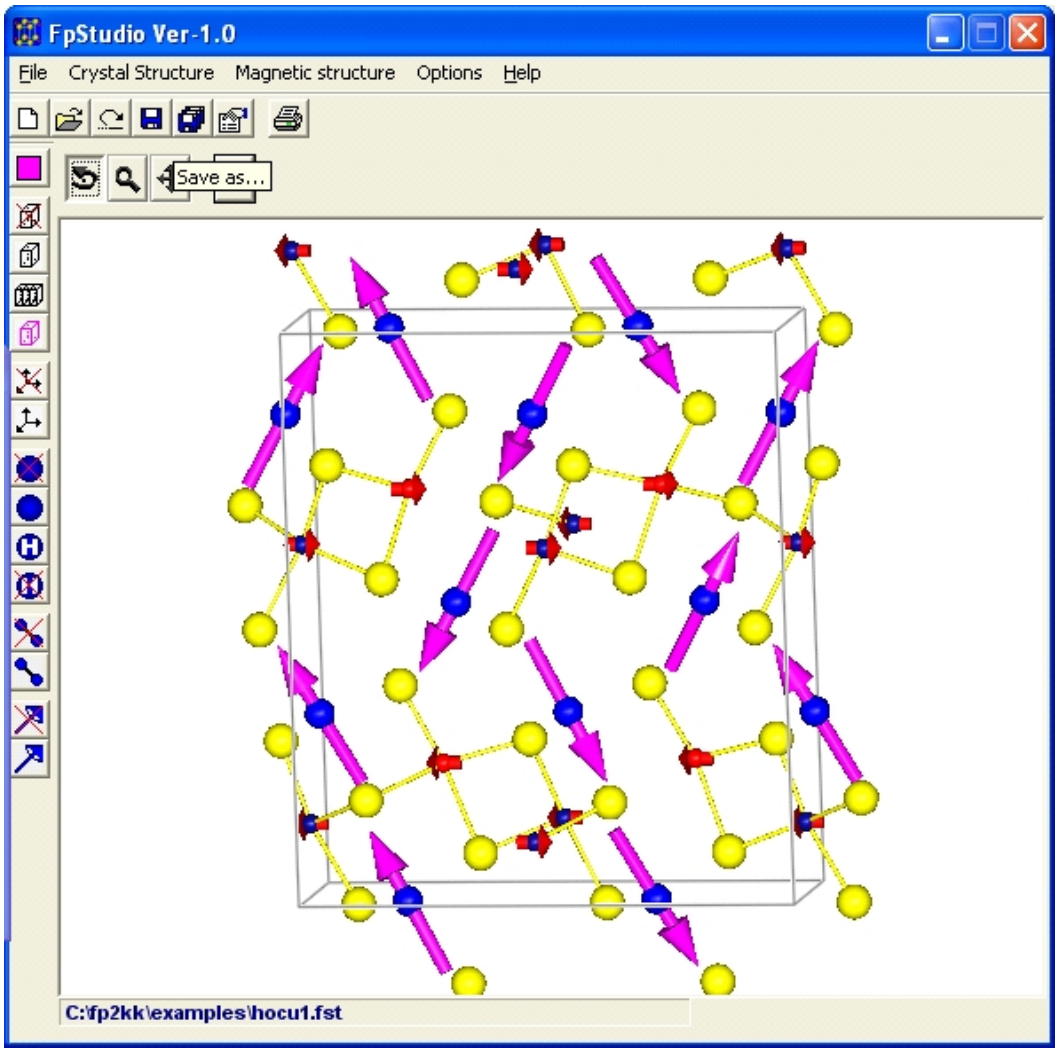
A block of symmetry operators similar to that appearing in the PCR file for a magnetic phase when Isym=-1.

Example for FST file

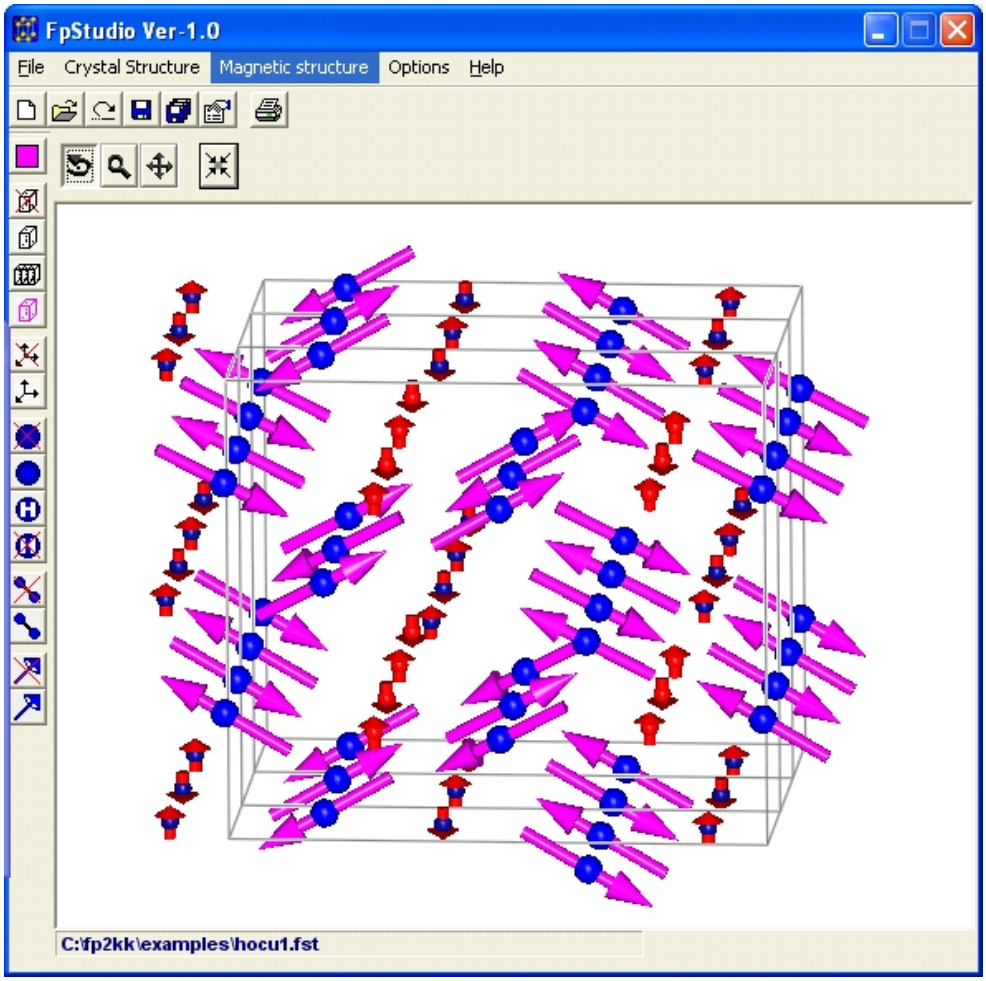
```
!Title: Something  Magph2
SPACEG P 6/m m m
CELL     5.206175    5.206175 8.149893  90.0000  90.0000 120.0000  DISPLAY MULTIPLE
BOX   -1.15  1.15   -1.15  1.15    -0.15  4.15
BKG  1 1 1 1
ATOM Dy    DY      0.00000  0.00000  0.00000
ATOM Mn    MN      0.50000  0.00000  0.25018
ATOM Ge1   GE      0.33333  0.66666  0.50000 nodisplay
ATOM Ge2   GE      0.33333  0.66666  0.00000 nodisplay
ATOM Ge3   GE      0.00000  0.00000  0.34428 nodisplay
CONN MN MN 0 3.2 COLOR 0 1 0 1

{
LATTICE P
K     0.00000   0.00000   0.00000
K     0.00000   0.00000   0.16558
SYMM   x, y, z
MSYM   u, v, w, 0.00
SYMM  -y, x-y, z
MSYM   u, v, w, 0.00
SYMM  -x+y, -x, z
MSYM   u, v, w, 0.00
MATOM Dy    DY      0.00000  0.00000  0.00000   GROUP    scale 0.6
SKP         1  1  0.00000  0.00000  4.10673    0.00000  0.00000  0.00000    0.00000
SKP         2  1 -6.25495  0.00000  0.00000   -3.61130 -7.22259  0.00000    0.00000
MATOM Mn1   MN      0.50000  0.00000  0.25024   GROUP
SKP         1  1  0.00000  0.00000 -1.14495    0.00000  0.00000  0.00000    0.00000
SKP         2  1 -1.75407  0.00000  0.00000   -1.01271 -2.02543  0.00000    0.47363
MATOM Mn2   MN     -0.50000  0.00000 -0.25024   GROUP
SKP         1  1  0.00000  0.00000 -1.14495    0.00000  0.00000  0.00000    0.00000
SKP         2  1 -1.75407  0.00000  0.00000   -1.01271 -2.02543  0.00000   -0.47363
}
```

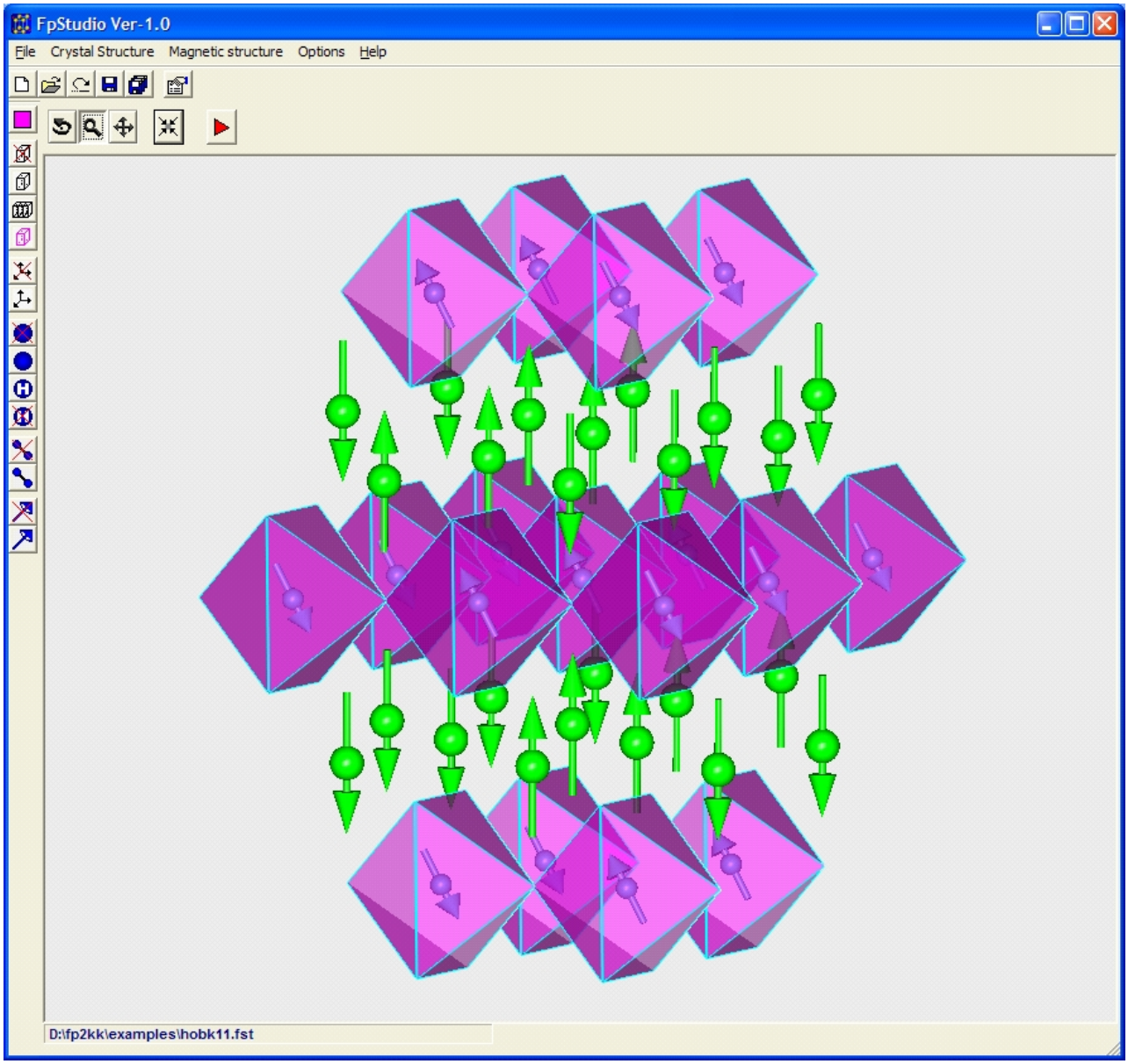
ScreenShots of FpStudio

The file "hocu.fst" is obtained directly by running FullProf on the example "hocu.pcr".



The next image has been obtained from the previous one by removing the bonds (clicking on the fourth button on the left starting from the bottom part), the oxygen atoms (yellow spheres, removed using the Atom sheet obtained by selecting it from the Crystal Structure menu) and adding two additional unit cells along the **b** axis (by increasing the Box limits, obtained from the Options menu).


FpStudio Ver-1.0
File
Crystal Structure
Magnetic structure
Options
Help
C:\fp2kk\examples\hocu1.fst



Screenshot of ***FpStudio*** showing a polyhedral representation of the crystal and magnetic structure of Ho_2BaNiO_5.

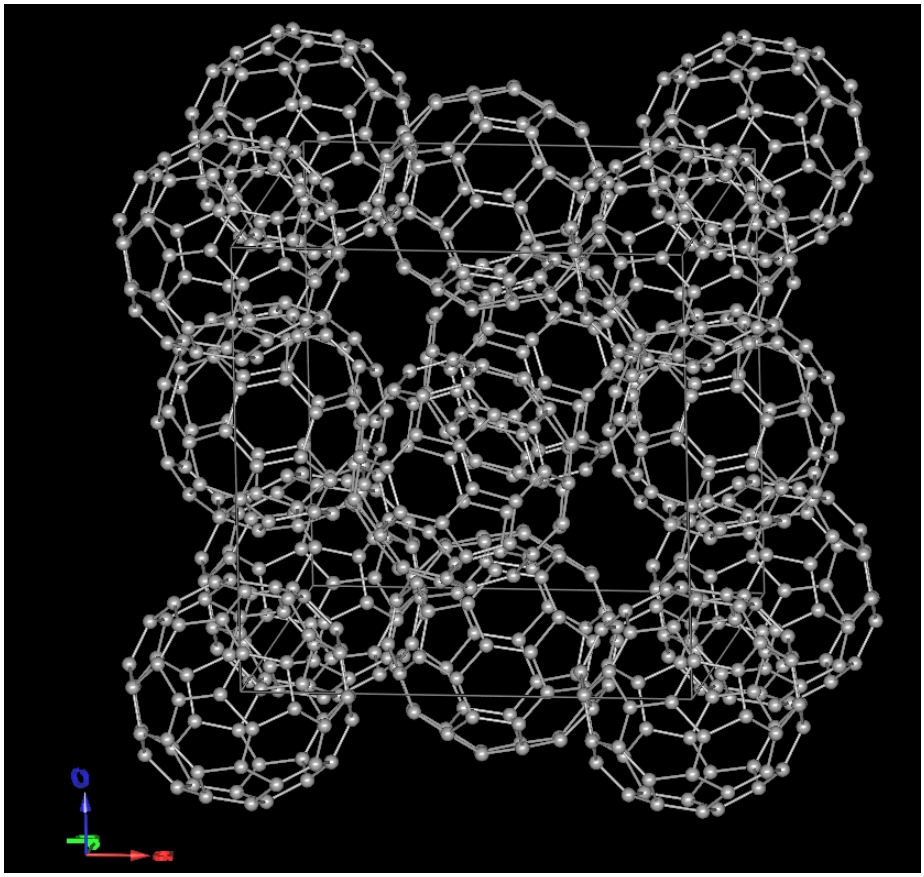


Image of C_{60} in its *Pa3* phase. This corresponds to a bitmap exported from FullProf Studio using the corresponding item in the File menu.

Additional notes

Notice that the keyword COLOR, within the PCR file, can be given an explicit name instead of a 4-dimensional vector (RGBT, for read, green, blue and transparency) within the PCR file. They are converted to numerical form before writing to the FST file.

The presently available colours are: BLACK, WHITE, YELLOW, RED, GREEN, BLUE, GREY, VIOLET, CYAN, BROWN, DARKGREEN, SEAGREEN, ORANGE, SALMON, PINK, DEEPPINK, MAGENTA, PURPLE, and GOLD.

In the PCR file the information contained in the keywords to be put in the atom lines must be given in the following order: first RADIUS/SCALE, second COLOR, last BOND or CONN. The colour of a bond must be given after BOND/CONN and the numerical form (R,G,B,T) is imperative. BOND and CONN cannot appear in the same PCR line. Most of the examples PCR files provided in the FullProf Suite have been modified in order to include keywords for witting the corresponding FST file.