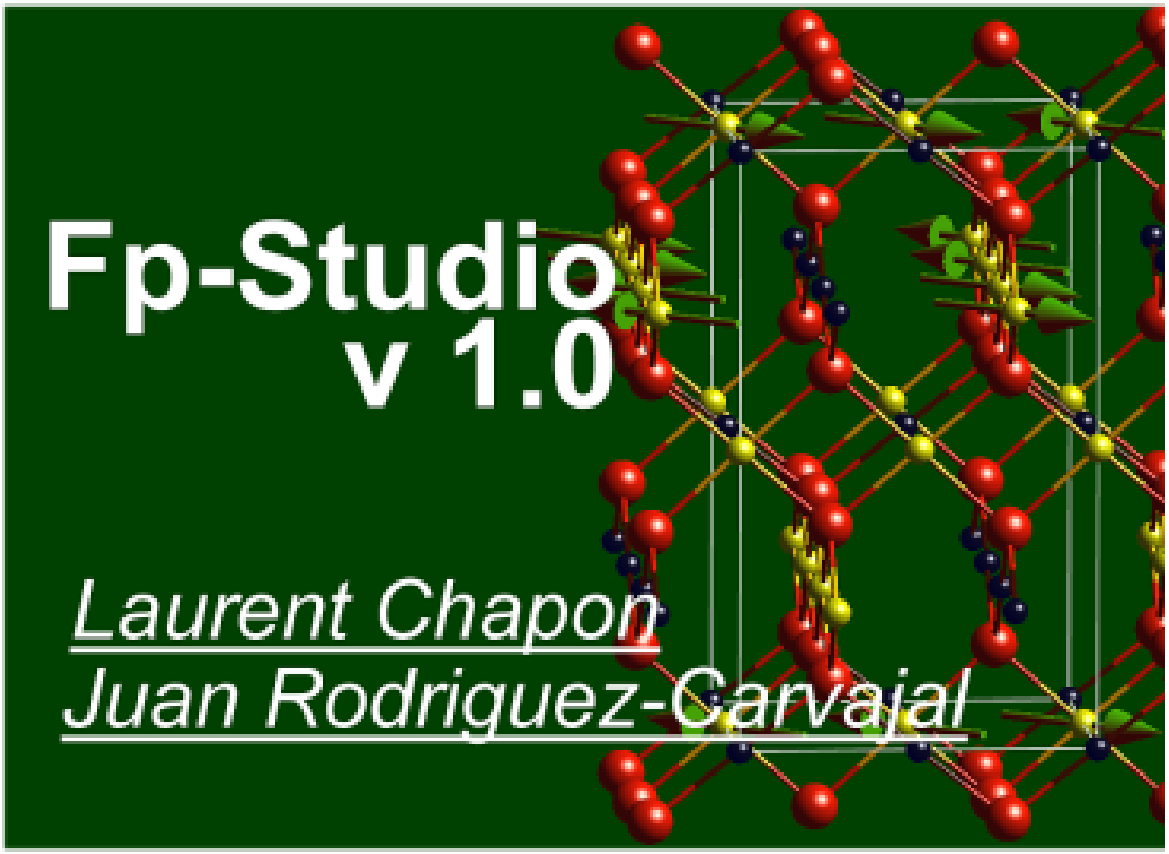

Manual of

FULLPROF STUDIO

(Version 1.0 November 2004)

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Introduction to FULLPROF STUDIO

The version 1.0 of the FULLPROF STUDIO program is being distributed with the current version of the FULLPROF SUITE. The program FULLPROF STUDIO 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 LLB (Saclay, 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.

At present the program is being strongly modified in order to incorporate new features. Here we give some of the most important keys for using the program.

Running FULLPROF STUDIO

A present the program runs on Windows and Linux platforms. Here we describe the use of FULLPROF STUDIO in a Windows platform.

- The program can be run from a DOS shell typing "fp_studio", clicking on its icon or from the "Studio" button in WINPLOTR. 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 FULLPROF STUDIO 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).

From the interface, clicking on the "open file" button or from the "open" item in the "File" menu, the user can open an FST file.

If there is no error the program opens a window with a plot of the structure that can be rotated with the help of the mouse. At present, the only way to save an image is by using the "prnt scrn" key and pasting it in a windows application (Power Point, Word, MSpaint, etc...). A bitmap can also be exported but currently a bug in the WINTERACTER library (when using OPENGL) produces the disappearance of the image after saving. The bitmap file is anyway generated correctly.

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

Controlling the input FST file from the PCR file

The current version of FULLPROF produces always an output for FULLPROF STUDIO, even if it is not explicitly asked by the user. Even in the case the user makes nothing to control the FST file, FULLPROF automatically generates a file that is readily useful for FULLPROF STUDIO. However, in order to get better results from the beginning the following prescriptions are recommended:

1. If a nuclear part is related to one or several magnetic phases the keywords `magphn` must appear in the line with the name of the phase. The final symbol `n` should be substituted by the numeral (integer) representing a magnetic phase related to the current crystallographic phase (e.g. `My_phase_name magph2 magph3`. This tells to the program to associate the magnetic phases 2 and 3 to the current crystallographic phase). The FST file corresponding to the nuclear phase contains all the magnetic information needed for visualisation. One can however visualise a pure magnetic phase but in this case the atoms are not visible. Only the arrow representing the magnetic moments can be visualised

2. The program generates automatically several keywords (see below), but additional plotting keywords can be added at the end of the atoms lines. To start the plotting keywords the symbol "#" is used. For instance, the directive "`# RADIUS 0.8 COLOR 1 0.2 0.2 1 BOND Cu1 Cu 0.0 2.3`" added in the same line of an atom at the end of the normal PCR line will create the appropriate keywords in the FST file. Remember that the `BOND` directive must appear after other keywords affecting the current atom. The `BOND` directive can make reference to different atoms. The keywords are case insensitive but not the label used for atoms.

There is another version of the program, called "fp_studio_dyn", that is useful for looking dynamically the behaviour of the structure during a refinement or a simulated annealing run. For that FULLPROF has to generate a *.fst file at each refinement (or Monte Carlo) cycle, this is obtained by putting the flag `Ls2 = 5` (LSQ refinement or Simulated Annealing job) in addition to `Jview=3`. In the case of a Simulated annealing job the name of the *.fst file is fixed to "simann.fst". One can run FULLPROF in a shell or from WINPLOTR and go, in a DOS shell, to the directory where the current files are read or written. Then type "fp_studio_dyn simann" to see the behaviour of the atoms during the structure solution process. FULLPROF and f_studio_dyn run simultaneously and the whole process is slower.

Content of the input file (FST file)

All lines starting with "!" are considered as comments. The file contents a list of keywords needed to plot the structure. For plotting a crystal structure the following keywords are needed:

`SPACEG` is followed by the Hermann-Mauguin symbol of the space group given in the same format as in FULLPROF (e.g. `SPACEG I 41/a m d`). 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, e.g. GENER x,-y,z+1/2. Up to 15 generators are allowed.

CELL is followed by six real numbers (a, b, c, alpha, beta, gamma) defining the cell parameters (e.g. CELL 4.32 4.32 8.41 90.0 90.0 90.0)

BOX is followed by six real numbers representing the volume of the structure to be considered for plot (BOX xmin xmax ymin ymax zmin zmax)
(E.g. BOX -0.15 1.15 -0.15 1.15 -1.25 1.25)

BKG This optional keyword must be followed by a legal colour value (see below). 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.

ROTAX This optional keyword and the forthcoming up to ATOM refer to the orientation view of the unit cell the first time the program is invoked. ROTAX is followed by four real numbers. The first (ang) is an angle in degrees and the other three represent the components of a unit vector in Cartesian coordinates around which a rotation is performed. The orientation of the system (if no orientation keyword is given) is a view along the c-axis with the a-axis horizontal and directed to the right. The values of ROTAX are output in the DOS-shell each time one changes the orientation of the view using the mouse. The user may copy and paste these values in the FST file for further processing. (e.g. ROTAX 288 1.0 0.0 0.0)

VIEW This is an optional keyword that is followed by three real values representing the vector (in Cartesian components) along which the structure will be output on the screen (e.g. "VIEW u v w", with u, v, w, real numbers, default VIEW 0 0 1)

SPHER Followed by two real numbers representing the spherical angles theta and phi of the orientation axis (the same as that given in VIEW, e.g. SPHER 87 10). It is also optional.

ROTXYZ Optional keyword followed by three real numbers representing the rotations (in degrees) along x, y and z to be applied to the default orientation in order to obtain the desired view. The rotations are applied in the following order first "rotx", then "roty" and, finally, "rotz". A point P is transformed to point P' as: P'= rotz(roty(rotx(P))). (e.g. rotxyz 88 10 0)

If several rotation instructions are given in the file, only the last one is applied in practice.

ATOM This keyword is followed by the label of the atom, the chemical symbol the fractional coordinates and, optionally, other keywords. The additional keywords are given for plotting purposes. At present they are: DISPLAY (default), NODISPLAY, RADIUS and COLOR (e.g. ATOM Cu1 CU 0.0 0.0 0.5 RADIUS 0.8 COLOR 0.8 0.8 0.1 1). The number of ATOM keywords is not limited.

BOND Optional keyword followed by two atom labels and two real numbers. The two numbers representing 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. 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
```

CONN This optional 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.

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

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 now given in a separate line from MATOM (see below). 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:

LATTICE This keyword is, normally, the lattice symbol of the Space group.
(E.g. LATTICE I)

K Followed by three real numbers representing the components of the propagation vector with respect to the reciprocal basis of the conventional unit cell (e.g. K 0.5 0.0 0.123). Several K keywords can appear in a single magnetic block.

SYMM and **MSYM**
A block of symmetry operators similar to that appearing in the PCR file for a magnetic phase when Isym=-1. An example is given below.

MATOM This is similar to ATOM keyword. The plotting keyword SCALE followed by a real value, can be added in order to re-scale the magnetic moments. The keyword GROUP can also be given after the fractional coordinates, telling to the program that the Fourier coefficients corresponding to different propagation vectors have to be grouped to calculate the total magnetic moment. If one prefers to represent the arrows corresponding to each propagation vector, the keyword GROUP should be removed. There's no limit for the number of MATOM lines.

The Fourier coefficients of the magnetic structure are written just following the MATOM lines in the following format:

SKP n1 n2 Rx Ry Rz Ix Iy Iz MPhas optional keywords

Where SKP is the keyword introducing the Fourier coefficients. The integers n1 and n2 correspond to the number of the propagation vector in the block and the number of magnetic

matrices to be applied (same meaning as in FULLPROF). The numerical values `Rx`, `Ry`, `Rz`, `Ix`, `Iy`, `Iz` and `MPhas` correspond to the following expression of the Fourier coefficients:

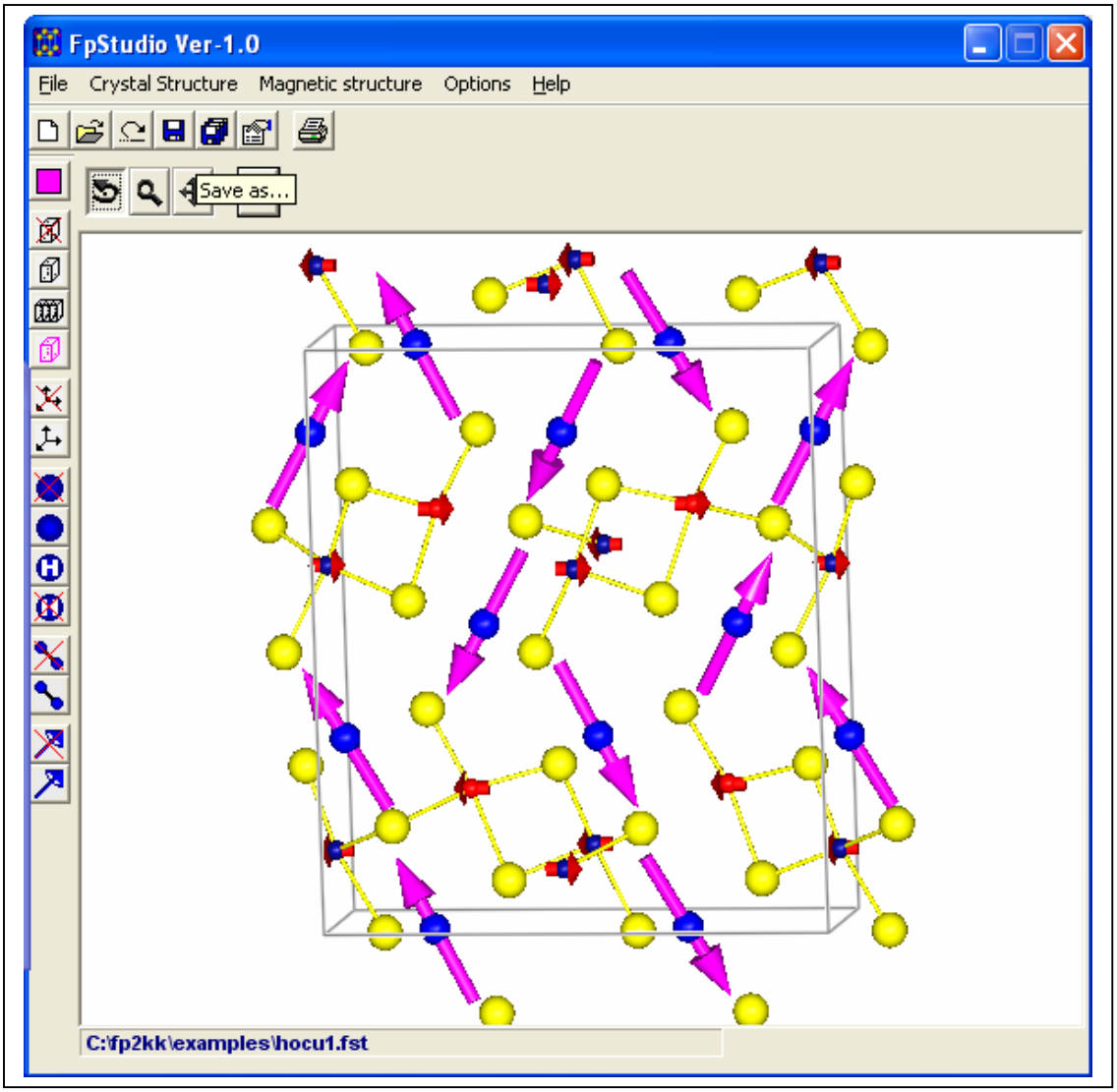
$$\mathbf{S_k} = \frac{1}{2}\{\mathbf{R} + i\ \mathbf{I}\}\exp(-2\pi i\ \phi)$$

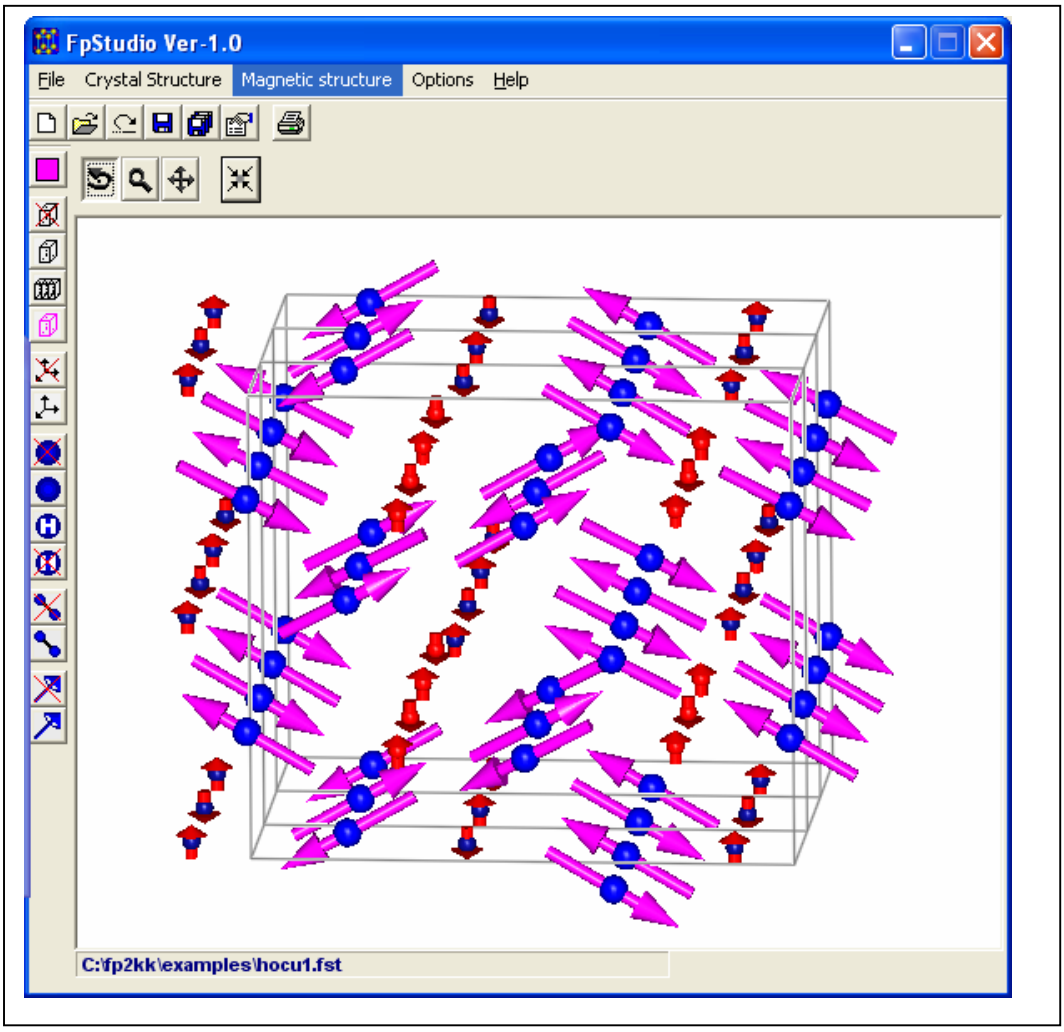
$$\mathbf{S_k} = \frac{1}{2}\{(R_x, R_y, R_z) + i\ (I_x, I_y, I_z)\}\exp(-2\pi i\ Mphas)$$

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

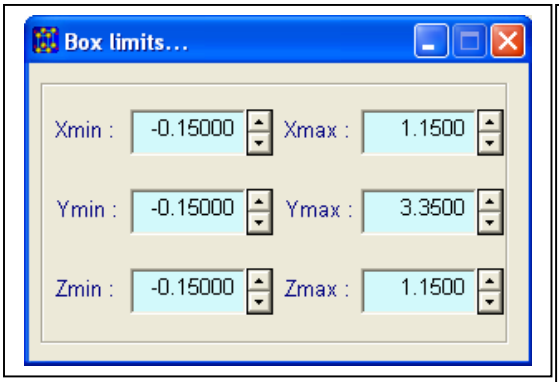
Screen Shots of FULLPROF STUDIO

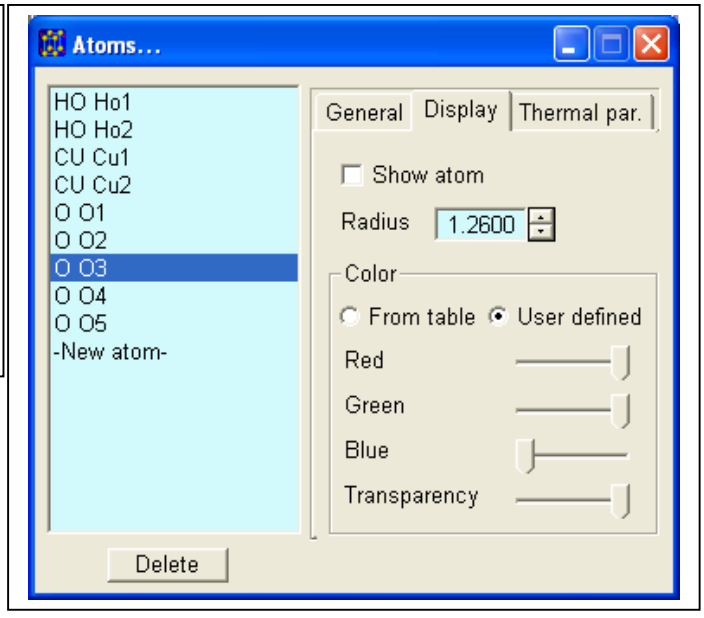
Below there is the image of FULLPROF STUDIO during a working session. The file "hocu.fst" is obtained directly by running FULLPROF on the example "hocu.pcr".





The image above 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).





The functionalities that are not completely available in the interface can be manually set by editing the FST file via a button in the interface.

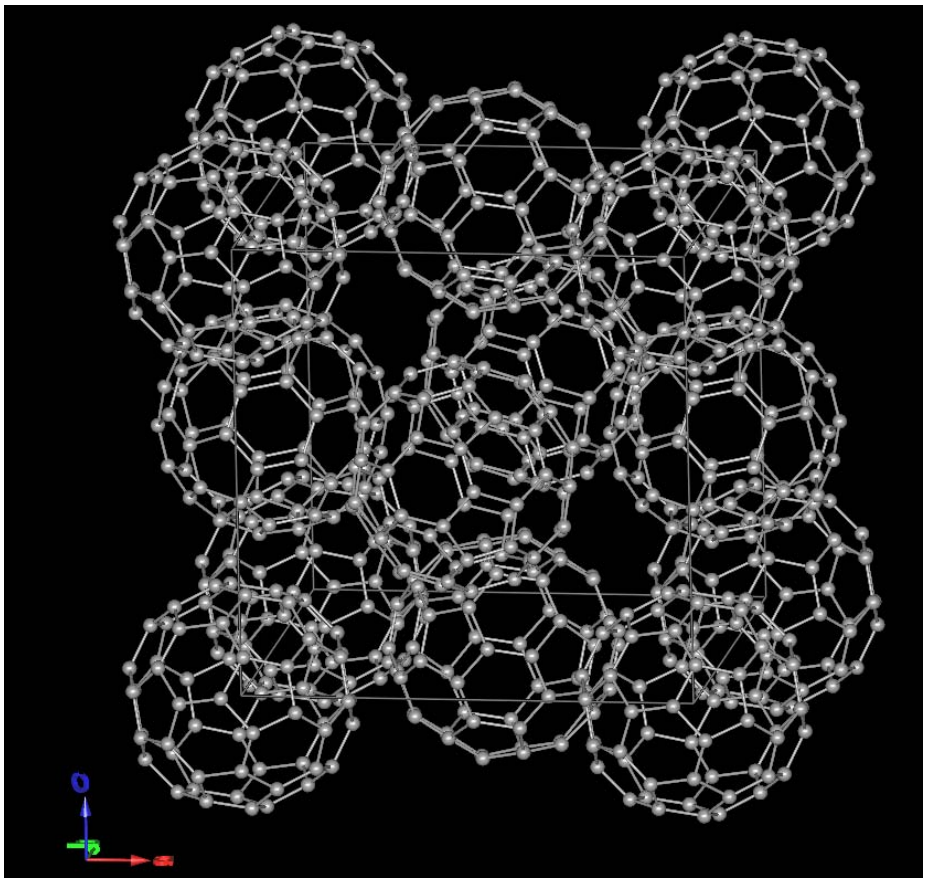


Image of C_{60} in its *Pa3* phase. This corresponds to a bitmap exported from FULLPROF STUDIO using the corresponding item in the File menu.

Additional notes

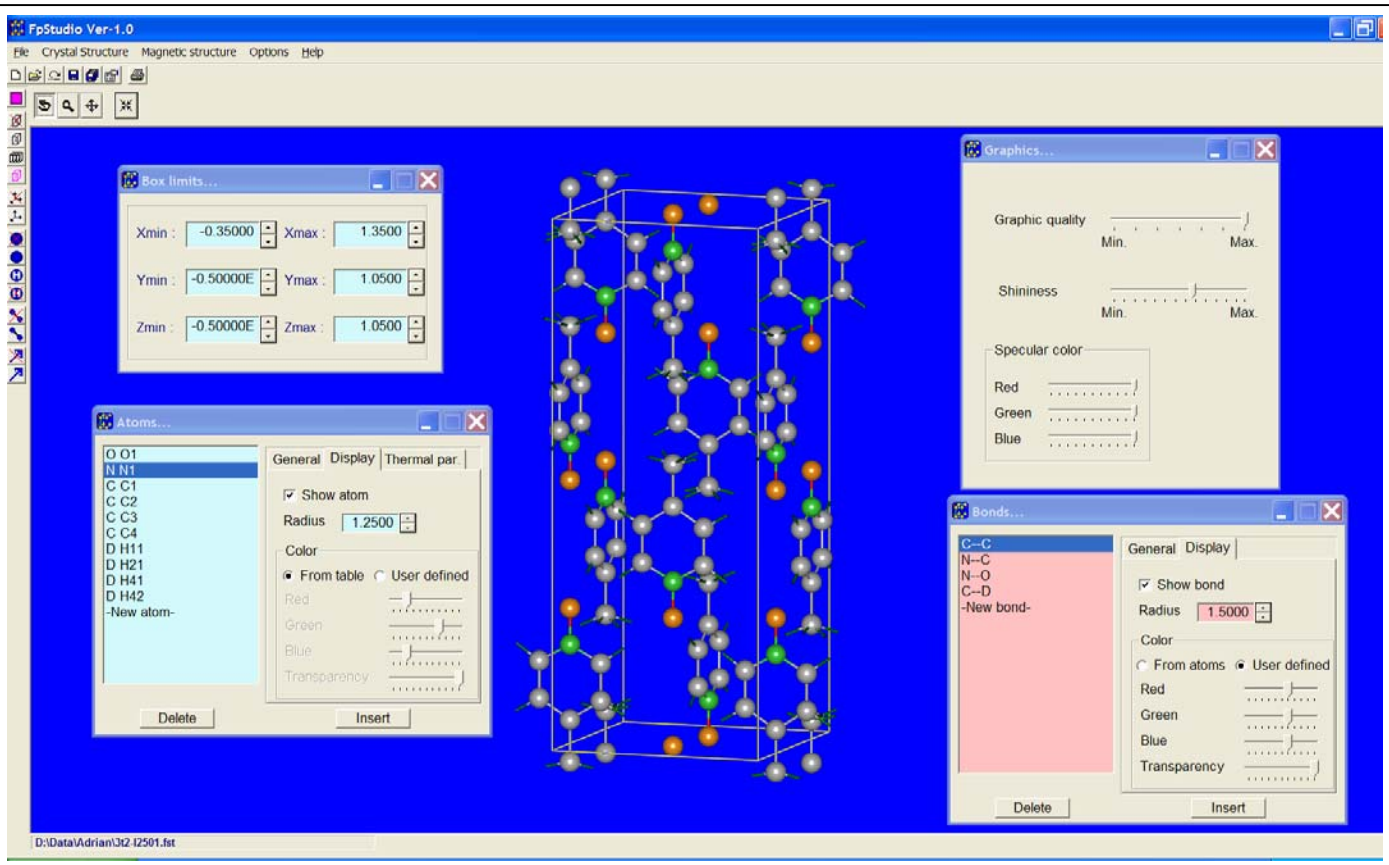
Notice that the keyword COLOR, within the PCR file, can be given an explicit name instead of a 4-dimensional vector (RGBT, for read, green, blue and transparency) within the PCR file. They are converted to numerical form before writing to the FST file. The presently available colours are: BLACK, WHITE,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

A complete example of FST file is given below.

```
!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
}
```



General view of a session of FULLPROF STUDIO on a molecular compound.