Xlens GUI Program

XLENS® - A computer program for solving crystal structures from single-crystal and powder diffraction data

XLENS is a program compiled with Lahey/Fujitsu Fortran 95 Compiler that can be used free for academic purposes. It is supported by the FULLPROF/WINPLOTR platform via compatible input and output files. Although XLENS/11 has been tested on a variety of compounds and space group symmetries, *the author has no liabilities in respect of errors in the program and documentation.*

Citation of the reference [Rius,J. (1993) *Acta Cryst.* A49, 406-409] would be greatly appreciated when publishing works done with it.

GXLENS Program

GXLENS is a GUI application to manage the input files for XLENS program. It is compiled using Lahey/Fujitsu Fortran 95 Compiler and Winteracter library (http://www.winteracter.com) and actually it is under development yet. The author is not responsible for erroneous results obtained with the program.

General Description

XLENS is a direct methods program that solves crystal structures from single-crystal (SC) or powder (PW) diffraction data. Ideally, the program works with the intensities of the unique reflections up to atomic resolution as well as with the approximate chemical composition of the compound. The program solves the crystal structure by optimising the phase values (generically denoted by Φ) of the large structure factors. In the solution of small crystal structures from SC data, this optimisation (phase refinement) is achieved by maximising the origin-free modulus sum function $S(\Phi)$ (Rius, 1993)

$$S(\Phi) = \langle [\ |E(\mathbf{H})| - |E|_{av}\ ] \cdot |E(\mathbf{H},\Phi)| \rangle_{\mathbf{H}} = \max.\ !$$

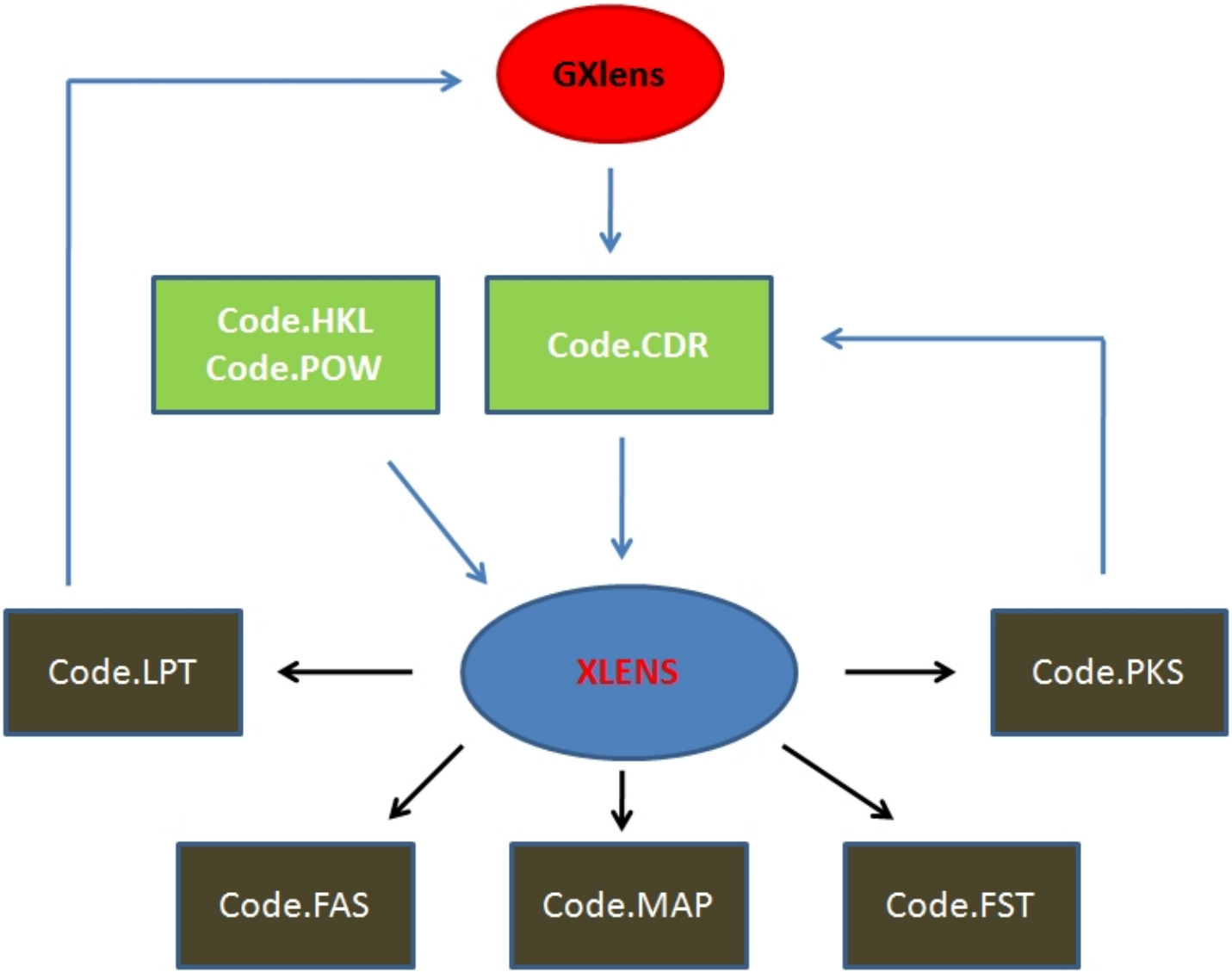
In this expression $|E(\mathbf{H})|$ are the moduli of the normalised structure factors of both large and weak reflections, $|E|_{av}$ is the average observed E value and $|E(\mathbf{H},\Phi)|$ are the moduli calculated in terms of the phases. The very robust phase refinement procedure implemented in this **XLENS** version uses the FFT algorithm and is called S-FFT (Rius et al., 2007).

In a typical default SC run, XLENS carries out 25 sets of phase refinements. Each set starts with random phase values for the large structure factors and ends with the refined phases Φ_{ref} that are used to compute the figure of merit (FOM) of each phase refinement trial. The FOM is the correlation coefficient between observed $|E(\mathbf{H})|$ and calculated $|E(\mathbf{H},\Phi)|$ moduli. After the phase refinement, the Fourier recycling part follows. This part ends with the calculation of a final R-value including all individual reflections. The structure solution process stops when at the end of the Fourier recycling the final R-value is lower that a preset value. Otherwise the next set of random phase values will be processed. XLENS can also develop and complete partial structures.

The PW case is normally more complicated. The PW peculiarities regarding file organisation (compatibility with the FULLPROF suite of programs) and specific strategies are described at the end of this WinHelp file.

FileOrganization

Select a code name for the compound to identify their data files. To run the program, introduce XLENS07 followed by this code (separated by a blank) in the command line. The I/O files of XLENS/XLENSG are shown in the diagram below.



Schematic diagram showing the file organization of XLENS

The two input files are code.CDR and code.HKL:

• **File code.CDR** contains the crystal data and the control parameters of the program and will be described in detail in the next section and you can use the XLENSG program to do an input file in easy way.
• **File code.HKL** includes the intensity data. Preferably only reflection data belonging to one asymmetrical unit of reciprocal space must be included with the systematically absent reflections removed. There must be one reflection per line. Reflections with negative F- or F2 values are skipped. The type of input format is indicated with the keyword IHKL in file code.CDR (see there for supported input formats). The internal structure of code.HKL is compatible with files *.HKL of the least-squares program SHELXL-93. File code.POW replaces code.HKL in the PW mode.

The output ASCII files are code.LPT, code.PKS, code.FAS, code.MAP and code.FST:
• **File code.LPT** is the printer output file with the complete results of the calculations. At the end it prints a copy of file code.CDR.
• **File code.PKS** contains the atomic coordinates of the solution with the lowest R-value.

- **File code.FAS.** For certain special applications it may be useful to have at one's disposal the refined phase values. These are written in this file.
- **File code.FST** is the input file for program FStudio (Crystal structure Drawing) in the FullProf Suite.
- **File code.MAP.** File with the Fourier map that can be directly processed either by program FAN of the FROG-PC series or program GFourier in the FullProf Suite.

Description of code.CDR

Mainly the input file for XLENS (code.CDR) has three parts:

1. Crystal data;
2. Control keywords;
3. Eventually, the atomic coordinates of the partial structure (or alternatively a set of phased reflections) for Fourier recycling or phase refinement.

A typical example of file code.CDR is

```
[pro-pro-phe-phe-gly-].MeOH.H20 in P212121; 86 atoms
CELL
13.999 21.602 21.615  90.  90.  90.
LATTICE
1
SYMMETRY
 X, Y, Z
-X+1/2, -Y, Z+1/2
-X, Y+1/2, -Z+1/2
 X+1/2, 1/2-Y,-Z
CONTENT
 6   248
 1   328
 7    40
 8    56
&CONTROL IHKL=1, NSET=200/
```

Title

Is the first line of the input file (code.CDR). It will contains an up-to-80-characters-long title with useful information. (compound name, chemical formula, space group symbol, number of molecules per unit cell and the date).

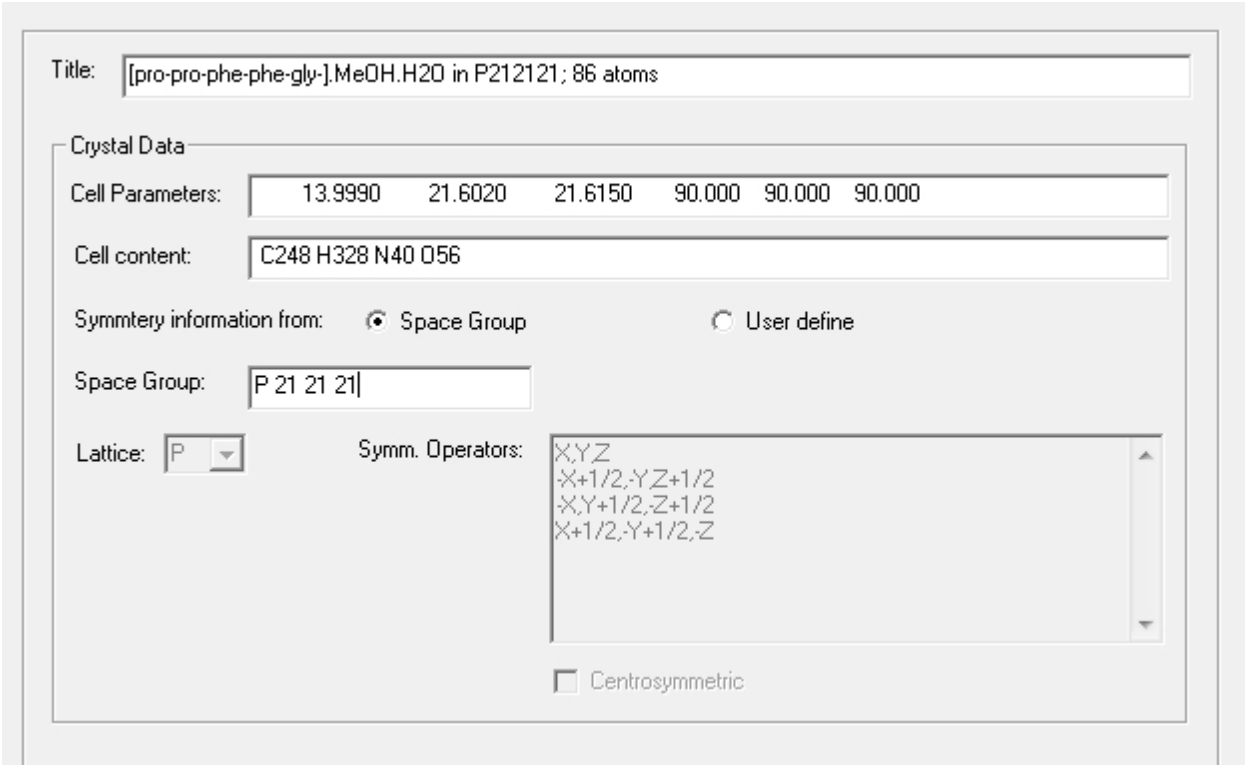
CrystalData

The remaining instructions of this part are recognized through the respective headings. Their order is indifferent. If one instruction contains more than one item, **these must be separated by blanks.**

keywords

CELL
LATTICE
SYMMETRY
CONTENT

All this keywords are shown in the next dialog of XLENSG program



Main differences between XLENS and XLENSG are:

Cell Content: In XLENSG the user write the Element symbol following by the total number of atoms of these species you have in the unit cell. Between different species you need introduce a blank character.

Symmetry information: In XLENSG program the user can select pass the information from the Hermann-Mauguin symbol (***Space group option***) or introducing directly the information about lattice, symmetry operators and centrosymetric case if the user select ***User define option***.

CELL

CELL
a b c α β γ

Cell dimensions. Lengths in Angstroms and angles in degrees.

CONTENT

CONTENT
Z1 N1
Z2 N2
...

Z1 and N1 are, respectively, the atomic number and the total number of atoms of type 1 in the unit cell, the same for type 2, etc. (maximum of 7 different atomic types).

For the special case of **neutrons**, enter Z = -1 for deuterium and Z= -5 for boron 11.

Important: The atomic type should be introduced in decreasing order of scattering power, i.e. heavy atoms before light ones. This data are used by the program to compute the internal **NCELL** parameter, i.e. the total number of atoms in the unit cell excluding H atoms.

LATTICE

LATTICE
n

n gives the lattice type (P=1, A=2, B=3, C=4, F=5, I=6 or R=7).
Default is n = 1.
If n is negative, the space group is treated as centrosymmetrical.

SYMMETRY

SYMMETRY
...line with one symmetry operator ...
...line with one symmetry operator ...

Each line contains one space group symmetry operation e.g.
X, Y, Z
1/2+X, 1/2-Y, -Z
...

The identity must be given as the first element. If the space group is centrosymmetrical, do not enter those symmetry operations generating equivalent positions related by the symmetry centre. For non-primitive space groups, only those symmetry elements associated with one lattice point are required. This instruction has no default values.

Control Parameters

The ***keywords*** controlling the different program options have **default values given in brackets**. For non default values, the keyword must be introduced in the CONTROL namelist that begins with **&CONTROL** and ends with **/.** A comma must always separate two keywords.

e.g.
&CONTROL IHKL=0, NSHELL=8/

For clarity, the keywords have been divided in various categories:

Input of Intensity data and Scaling
S-FFT Phase refinement
Automated Fourier recycling after S-FFT
Angles and distances among peaks in the Fourier synthesis
Input of Previously Known information

Intensity Data / Scaling

The intensity data are in file ***code.HKL***.

The observations can be either the structure factor moduli ***F*** or the squared moduli F^2 using the keyword **IHKL**. A reflection is observed if Fo > **FACDF**·σ(Fo) (or $Fo^2 > 2 \cdot$ **FACDF**$\cdot\ \sigma(Fo^2)$. The variable DSMIN is the minimum *d*-spacing of the input data set.

The relation between the quasi-normalised structure factor **E**, the scaling factor (**SK**) and the overall thermal vibration coefficient (**BO**) is given by the next equation:

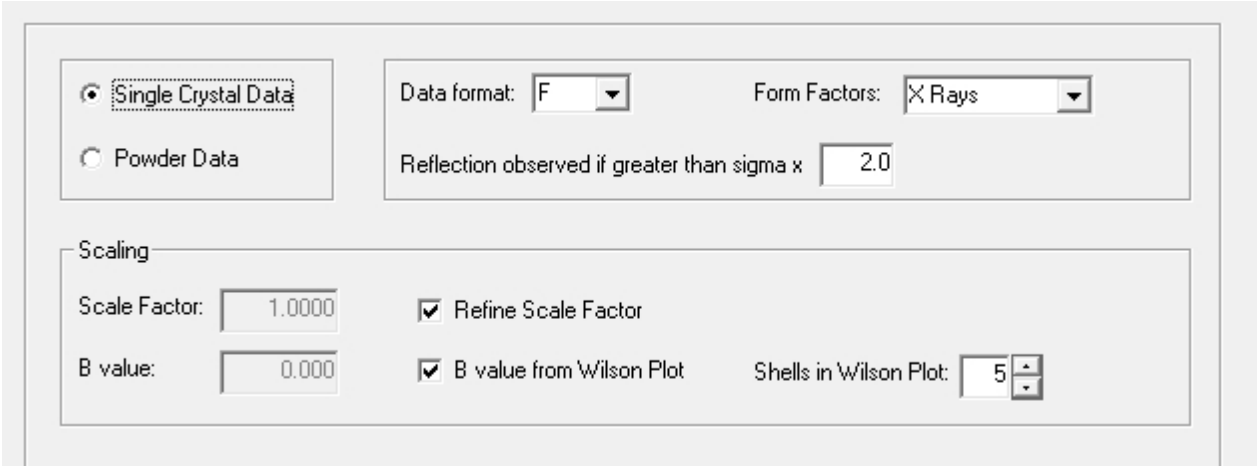
$$E(\mathbf{H}) = [F_{obs}(\mathbf{H})/SK] \cdot \exp[BO \cdot \sin^2(\theta_{\mathbf{H}}/\lambda)] / \mathrm{sqrt}[\Sigma f_{\mathbf{H}}{}^2]$$

keywords

IPOW

IHKL
FACDF
ISK
IBO
SK
BO
IFFORM
NSHELL

All these keywords are showed in the XLENSG program in the respective dialog when the user select the Intensity Data / Scaling button and the the program show the next dialog



BO

Keyword	***Input Variable***
BK=[3.0]	BO in $Å^2$

FACDF

Keyword	***Input Variable***
FACDF=[2.0]	A reflection is observed if Fo > FACDF·σ(Fo) (or Fo^2 > 2·FACDF· σ(Fo^2))

IBO

Keyword	***Input Variable***
IBO=[1]	BO is estimated from Wilson plot
= 0	Input BO value is not refined

IFFORM

Keyword	***Input Variable***
IFFORM=[0]	Form factor for X-rays
= 1	Fermi lengths for Neutrons
= 2	Form factor for Electrons

IHKL

Keyword	***Input Variable***	***Format***

IHKL=[0]	h k l F σ(F)	free (3I5, 2F12.2)
= 1	h k l F^2 σ(F^2)	free (3I5, 2F12.2)

IPOW

Keyword	***Input Variable***
IPOW=[0]	Single Crystal Data
= 1	Powder Data

ISK

Keyword	***Input Variable***
ISK=[1]	Scale factor SK is refined
= 0	Input SK is not refined

NSHELL

Keyword	***Input Variable***
NSHELL=[5]	Number of shells used in the Wilson plot (max. is 10)

SK

Keyword	***Input Variable***
SK=value	Scale factor

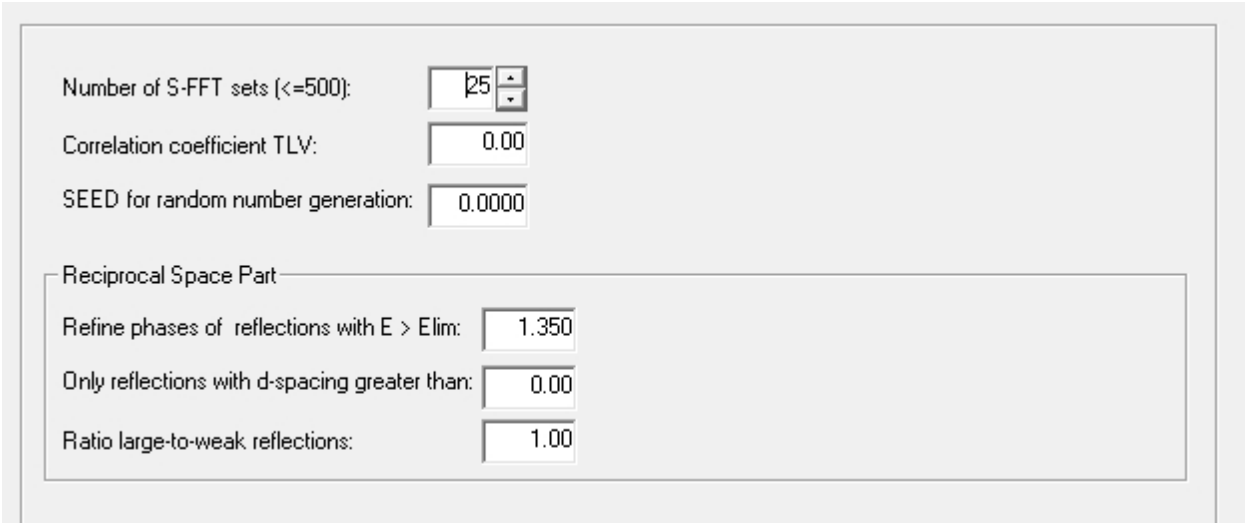
S-FFT Refinement

An alternative way of refining phases with the origin-free modulus sum function S is shown that, instead of applying the tangent formula in sequential mode, applies it in parallel mode with the help of the fast Fourier transform (FFT) algorithm. The main control parameters of this procedure are:

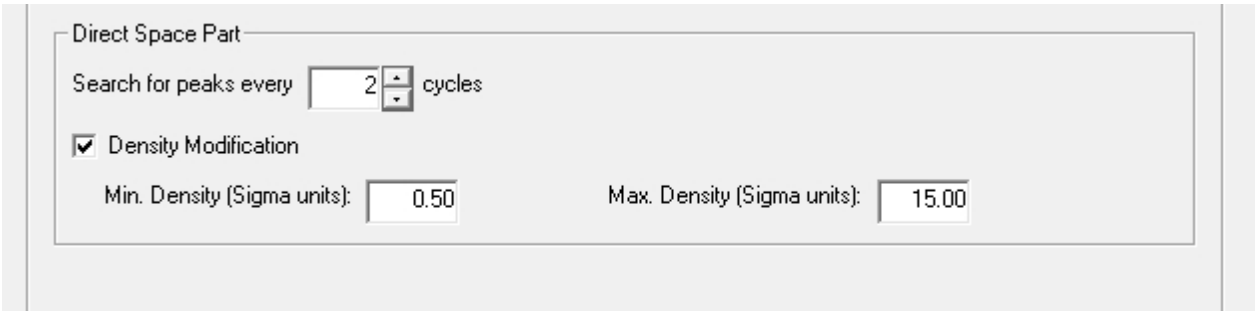
keywords

ELIM
DSDM
ERATIO
CCTLV
NSET
BINIT

The respective dialog in the XLENSG program is showed when the user select the next button



This dailog will show a Direct Space information if the user is working with Powder data.



BINIT

Keyword	*Input Variable*
BINIT=[0]	SEED for random number generation. Random numbers yield the initial phase values.

CCTLV

Keyword	*Input Variable*
CCTLV=[0.0]	Correlation coefficient threshold limit value. Direct methods solutions with values lower than CCTLV are not worked out. CC is defined in Rius et al. (2007)

DSDM

Keyword	*Input Variable*
DSDM=[0.0]	Only reflections with *d*-spacings (Å) greater than DSDM take part in the S-FFT refinement. Together with ELIM, it fixes the number of large reflections NLARGE. Notice that if zero, then DSDM = DSFOU

ELIM

Keyword	*Input Variable*
ELIM=[1.35]	Only phase values for reflections with |E| > ELIM. (|E| is the normalized s.f.)

ERATIO

Keyword	*Input Variable*

ERATIO=[X]	Number of weak reflections to number of large reflections used by the sum function.Default for single crystal is X=[NLARGE-SQRT(NLARGE)] / NLARGE.

NEGPKS

Keyword	*Input Variable*
NEGPKS=[0]	Positivity constraint in S-FFT and Fourier recycling.
= 1	no positivity constraint in S-FFT. That is the case for neutron data with negative scatterers and also for Fourier recycling handling positive and negative peaks

NSET

Keyword	*Input Variable*
NSET=[25]	Number of refined sets of random phases.
= 1	Normally used in combination with the BINIT value of a selected solution. (BINIT=seed of random number generator)

ROTLV

Keyword	*Input Variable*
ROTLV=[2.5]	Only active for NEGPKS= 1. It indicates the threshold limit of the peaks in the density function, i.e. ROTLV · σ(ρ).

Automated Fourier recycling

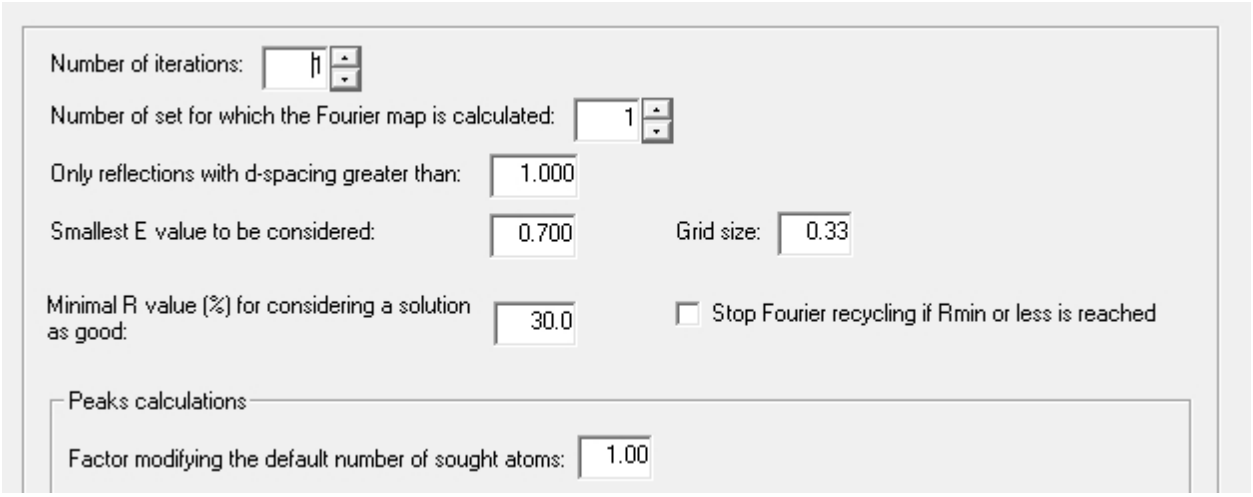
The main control variables for this part are:

keywords

DSFOU
ETRUNC
GRID
NITER
NMAP
RVMIN
IRVOUT
EXFAC
PEQ

Selecting the 

button, XLENSG show the next dialog to show the above parameters control. Here we are showing the part of dialog that correspond with these control parameters.



DSFOU

Keyword	*Input Variable*
DSFOU=[0.0]	Only reflections with *d*-spacings (Å) greater than DSFOU are considered by the Fourier part of the program. Notice that if zero, then DSFOU = DSMIN

ETRUNC

Keyword	*Input Variable*
ETRUNC=[0.7]	ξ values less than ETRUNC are ignored in the Fourier synthesis.

EXFAC

Keyword	*Input Variable*
EXFAC=[1.2]	EXFAC · NCELL is the number of atoms sought by the peak search subroutine. NCELL is the number of non-H atoms in the unit CELL.

GRID

Keyword	*Input Variable*
GRID=[0.33]	Grid size in Å. To save time, it can be increased but always < 1/3 * DSFOU.

IRVOUT

Keyword	*Input Variable*
IRVOUT=[0]	Non stop in Fourier- recycling.
= 1	Fourier-recycling stops as soon as a given cycle produces a solution with an R value lower than RVMIN

NITER

Keyword	*Input Variable*
NITER=[10]	Number of iterations in the recycling procedure.
= 1	the E-map is computed directly with the phases from S-FFT.

NMAP

Keyword	*Input Variable*

NMAP=[1]	Number of the solution for which the Fourier map is wanted. Default is the first solution

PEQ

Keyword	***Input Variable***
PEQ=[0.33]	Peaks closer than PEQ Å are considered equivalent by the peak search subroutine

RVMIN

Keyword	***Input Variable***
RVMIN=[30.]	Minimum R value to consider a solution as correct and to perform the peak search.

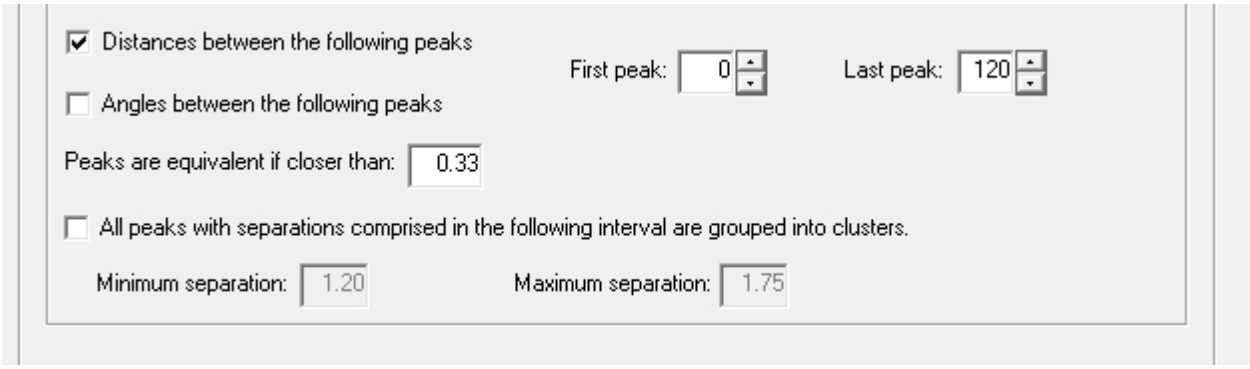
Angles and distances among Peaks in Fourier synthesis

Geomtric calculation can be done with the peak list found after Fourier synthesis process. The next keywords are used for this purporses.

keywords

IDIST
IANG
IFIRST
ILAST
ICONN
SEPMIN
SEPMAX

In the XLENSG program all these parameters are in the Fourier Recycling Dialog.



IANG

Keyword	***Input Variable***
IANG=[0]	
= 1	Angles are also calculated for the list peak

ICONN

Keyword	***Input Variable***
ICONN=[0]	
= 1	all atoms with interatomic separations less than SEPMAX are grouped into clusters.

IDIST

Keyword	*Input Variable*
IDIST=[0]	
= 1	Distances between found peaks are computed.

IFIRST

Keyword	*Input Variable*
IFIRST=[0]	Define the first peak on the lsit to be considered.

ILAST

Keyword	*Input Variable*
ILAST=[ALL]	Define the last peak on the list.

SEPMAX

Keyword	*Input Variable*
SEPMAX=[1.75]	maximum interpeak separations

SEPMIN

Keyword	*Input Variable*
SEPMIN=[1.20]	Minimum and maximum interpeak

Previous known information

XLENS program can handle two types of previously know information: located atoms (partial model) or phased reflections. For it we need tou use the **KARLE** keyword. In the last case, the known phase values are readen and kept fixed during the S-FFT refinement.

It is not possible to introduce a partial model and a set of known phases simultaneously!

Partial model
Known phase values

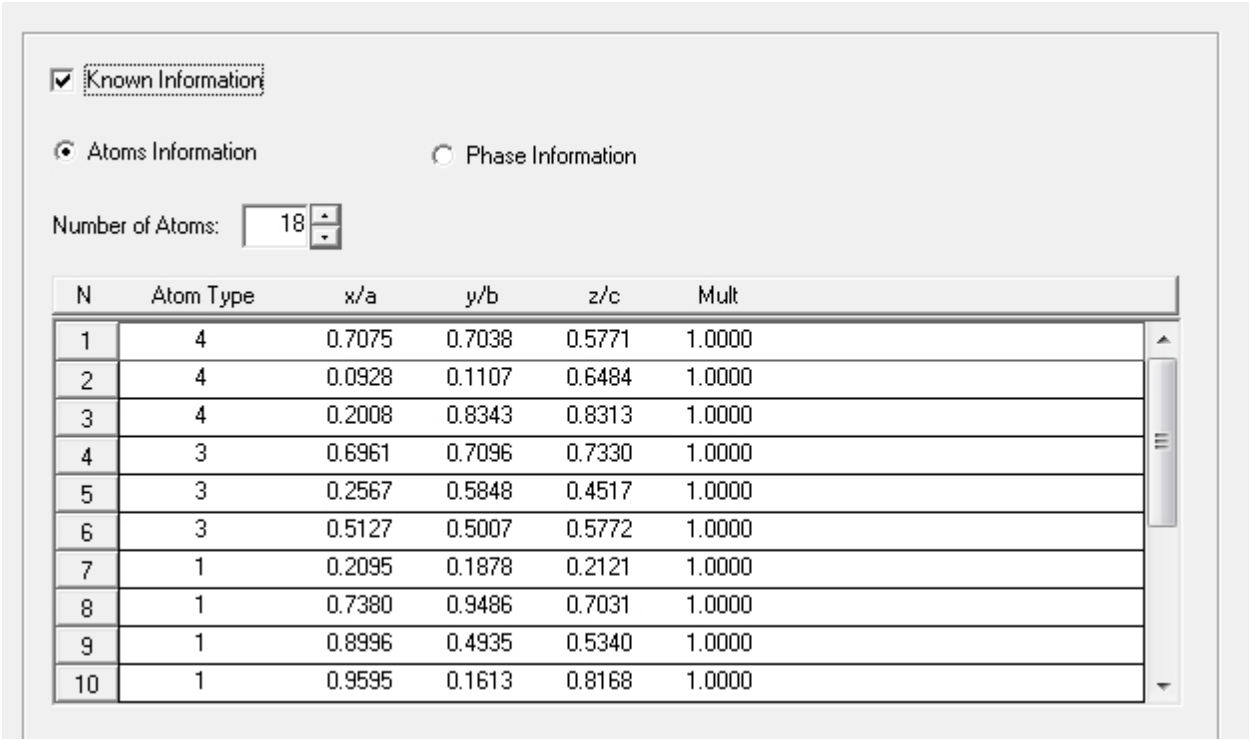
Keyword

KARLE
DSFX

XLENSG program show this part in the next dialog when 

is selected. Then the program show a particular dialog depending if the user select a partial model or mask phased reflections.

Here this an example for the MODEL case.



N	Atom Type	x/a	y/b	z/c	Mult
1	4	0.7075	0.7038	0.5771	1.0000
2	4	0.0928	0.1107	0.6484	1.0000
3	4	0.2008	0.8343	0.8313	1.0000
4	3	0.6961	0.7096	0.7330	1.0000
5	3	0.2567	0.5848	0.4517	1.0000
6	3	0.5127	0.5007	0.5772	1.0000
7	1	0.2095	0.1878	0.2121	1.0000
8	1	0.7380	0.9486	0.7031	1.0000
9	1	0.8996	0.4935	0.5340	1.0000
10	1	0.9595	0.1613	0.8168	1.0000

DSMSK

Keyword	***Input Variable***
DSFX=[0.25]	The lowest *d*-spacing of the reflections to be considered in FIXED

IFOU

Keyword	***Input Variable***
IFOU=[0]	No Fourier refinement
= 1	The partial model is read and the phase refinement for Fourier recycling. The partial model is headed with the word MODEL. (Only SC mode).

KARLE

Keyword	***Input Variable***
KARLE=[0]	
= 1	Using known information as MODEL or FIXED in the S-FFT phase refinement procedure. It is is valid for both modes SC and PW.

Partial model

The partial model is introduced in file code.CDR after the CONTROL namelist according to the following format:

1/ line: **MODEL**
2/ line: Number of lines with atom coordinates
3/ line and following ones: Atomic coordinates (one line per atom).

The required information for each atom is atomic type, x/a, y/b, z/c, multiplicity (free format).

If necessary, additional information can be written after the multiplicity. The program will ignore this information. A minus sign before the atomic type causes this particular atom to be not considered.

Known phase values

These are also placed after the CONTROL namelist according to the format:

1/ line: **FIXED**
2/ line: Number of lines containing phases
3/ line and following ones: h k l F phase_value (one line per phase).

The phase_value must be given in degrees and as an integer (free format).

A minus sign before the structure factor F causes this phase to be not considered.

Output files

XLENS produce a code.LPT containing the program results that you can see using an ASCII editor or select the  editor button on the toolbar of XLENSG program.

The following files can be also created.

File code.PKS

This file contains the atomic peaks found by the peak search subroutine. The internal structure of the file is:

1. line: TITLE
2. line: number of lines with atomic coordinates.
3. line and following ones: Atomic coordinates.

The required information for each atom (one line per atom) is,

atomic-type x y z multiplicity (free format)

A minus sign before the atomic type causes this atom to be ignored. Alternatively, the number of lines (or atoms) to be read can be reduced by changing the number in the second line.

File code.PKS can be included in file code.CDR for Karle-recycling (KARLE=1) or for Fourier refinement (IFOU=1). Notice that the first line must begin with MODEL.

File code.FAS

This file contains the refined phase values. The internal structure is:

1. line: number of refined phases Format: I8
2. line and following ones: h k l En(H) phi(H) Format: 3I4,F10.2,I5

En is the quasi-normalised E-value and phi the refined phase value.

File code.MAP

This file contains the Fourier map of the NMAP solution. This file can be directly processed by two programs for visual inspection:

a) *Program FAN of the FROG-PC series of programs for electron-density and model investigations for proteins* [Vernoslova,E.A. & Lunin,V.Yu. Inst. of Mathematical Problems of Biology, Pushchino (Russia). J.Appl. Cryst. (1993), 26, 291-294]. The internal structure of the formatted code.MAP file is:

1. line: '$$GA','X','Y','Z',' A'
2. line: ' FOURIER-MAP FROM XLENS'
3. line: A1,B1,C1,ALFA,BETA,GAMMA (= unit cell parameters; Format 6G10.4)
4. line: NXMX,NYMX,NZMX,M1,NXMX-1,M2,NYMX-1,M3,NZMX-1

(NXMX, NYMX, NZMX are the number of grid points in the x, y and z directions respectively; M1 = M2= M3 =0; Format 9I5)

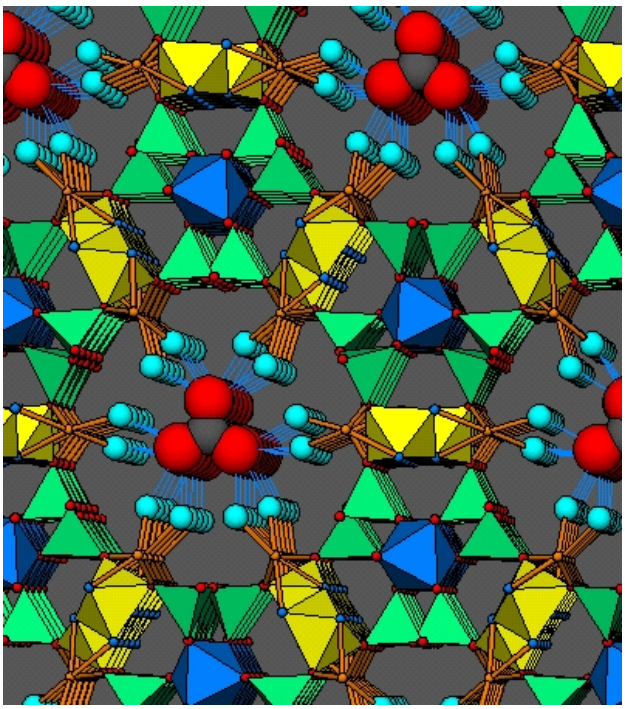
Next lines:
DO IZ=0,NZMX-1
((Z(IX,IY),IX=0,NXMX-1),IY=0,NYMX-1)
END DO

wherein Z is the matrix (0:127,0:127) with the function values; Format 9G10.4.

b*) The Program GFourier of the FullProf Suite recognises file code.MAP .* It is able to represent graphically the Fourier map.

File code.FST

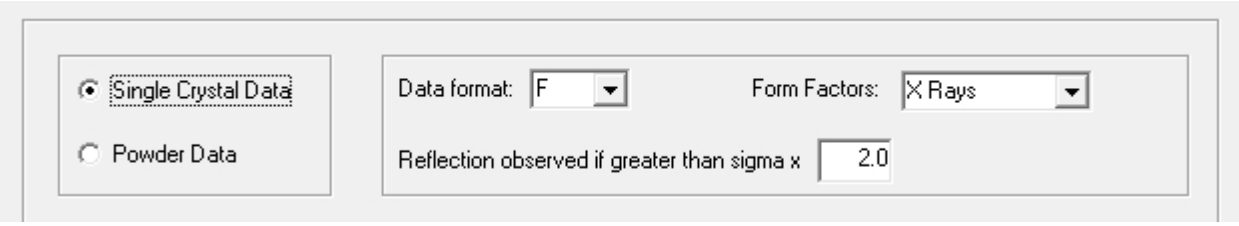
This is the input file for program FStudio, a program in the FullProf Suite for the graphical representation of atoms in the unit cell. The peaks found by XLENS in the Fourier map are ordered in decreasing height and assigned to atomic types according to the order specified in CONTENTS. In difficult cases it is advisable to check that the assigned atomic types are consistent with the peak heights. The two values written behind the peak coordinates are the peak height (normalised to 1000 for the largest peak) and the peak multiplicity, respectively.



Crystal structure of aerinite, a pyroxene-like mineral used as blue pigment in the romanic frescos of the Catalan Pirenees. The structure was solved with XLENS from synchrotron powder diffraction data.

Xlens for Powder Data

The powder diffraction part of **XLENS** is activated with the control parameter **IPOW.** This keyword is showed in the Intensity Data Dialog in the GXLENS program.



When **IPOW=1** the input file with the intensity data is not ***code.HKL*** but ***code.POW***. The internal structure (code.POW) is described in the next section. The general strategy when working with powder data is slightly different as for the ***SC*** mode due to the difficulty to preset the minimum R value (**RVMIN**).

In the ***PW*** mode it is better to run first all the **NSET** trials (e.g. 50 or 100), then to analise the different solutions for the one with the lowest R-value and finally develop this solution with an additional XLENS run. To be sure that all **NSET** trials are computed in the first run, **RVMIN** must be set very low, e.g. RVMIN = 1.

The Powder Data has also consequences on the control parameters, either by changing the default values:

ELIM	= [1.15]	
ERATIO	= [1.05]	
DSFOU	= [minimum *d*-spacing used]	The data resolution limit of the S-FFT parts is controlled with the unique keyword DSFOU (i.e. DSDM is no longer active).
NITER	= [1]	In the PW mode NITER is fixed to 1, i.e. the set of phases refined with S-FFT are directly used to find the listed atomic positions.
EXFAC	= [1.0]	EXFAC · NCELL is the number of atoms sought in the last peak search. In SC, NCELL is the number of non-H atoms in the unit CELL (see CONTENT instruction). In the PW mode NCELL can be modified by the user as explained below.
NSET	= [50]	

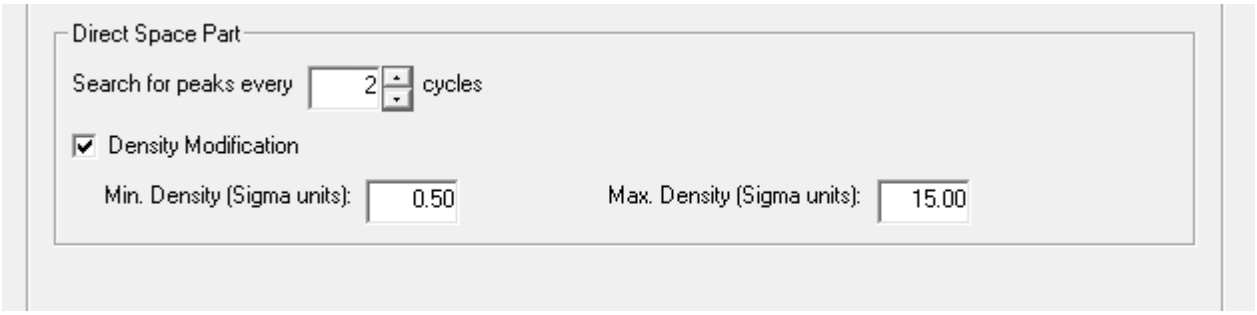
or by introducing new keywords.

When working with powder data, atomic resolution is seldom reached. In such cases the GRID parameter can be slightly increased (<0.33 * DSFOU) to speed up the calculations.

Keywords

IRODM
ROCUTL
ROCUTH
NCELL
IPICUP

All previous parameters are showed in the S-FFT Dialog when the user select the Powder data option in the Intensity dailog.



IPICUP

Keyword	*Input Variable*
IPICUP=[2]	Search of 'atomic' peaks in S-FFT refinement every IPICUP cycles. If very large, e.g. 1000, no peak search is performed.

IRODM

Keyword	*Input Variable*
IRODM=[1]	The electron density ρ is modified according to $\rho = 0$ for $\rho < \text{ROCUTL} \cdot \sigma(\rho)$ $\rho = \text{ROCUTH} \cdot \sigma(\rho)$ for $\rho > \text{ROCUTH} \cdot \sigma(\rho)$ [$\sigma(\rho)$ is the standard deviation of ρ]
= 0	

NCELL

Keyword	*Input Variable*
NCELL=[value]	NCELL is the number of (atomic) peaks in the unit cell used as real-space constraint in the algorithm. By default the value resulting from the CONTENT instruction is used. To exclude light atoms a value of NCELL equal to the number of dominating atoms in the unit cell can be introduced. Notice that for IPOW=1, EXFAC multiplies NCELL.

ROCUTL

Keyword	*Input Variable*
ROCUTL=[0.5]	See IRODM

ROCUTH

Keyword	*Input Variable*
ROCUTH=[15.0]	See IRODM

Internal structure of code.POW

This file contains the information of the observed powder diffraction pattern as processed by **XLENS**. This file can be created by running a profile matching (Le Bail) refinement with **FULLPROF** (option: More=1 and Jvi=12). The information for each reflection (one line per reflection) is:

```
IH IK IL FOBS MULT NVEI NGRUP THETA2 DC WT
(3I4, F16.4, 2I3, I5, F8.3, F11.5, F9.5)
```

The variables *IH, IK, IL, MULT, THETA2, DC* and *WT* are, respectively, the Miller indices, the multiplicity, the calculated 2-theta, *d*-spacing values and Bragg peak width (FWHM). For convenience, the reflections are ordered with increasing 2-theta values.

NGRUP is 1 if a reflection is well resolved from the previous one and 0 if it is overlapped, e.g. the sequence 1 1 **1 0 0** 1 1 indicates 2 resolved reflections, 1 group with three reflections (in bold) and 2 groups more with one reflection each one. This nomenclature allows the easy status modification of one reflection.

NVEI is the number of reflections in each group. If there is no overlap the group will consist of only one reflection, so that NVEI=1.

FOBS is the square root of the total intensity of the group. Consequently, all reflections of the same group have the same FOBS value.

References

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XLENS Program

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