CheckGroup

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Space group determination from powder diffraction pattern.

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Introduction

This program reads a file "codfiln.hkl" coming from *FullProf* when run on profile matching (Le Bail) mode and generates a list of possible space groups compatible with the observed diffraction pattern.
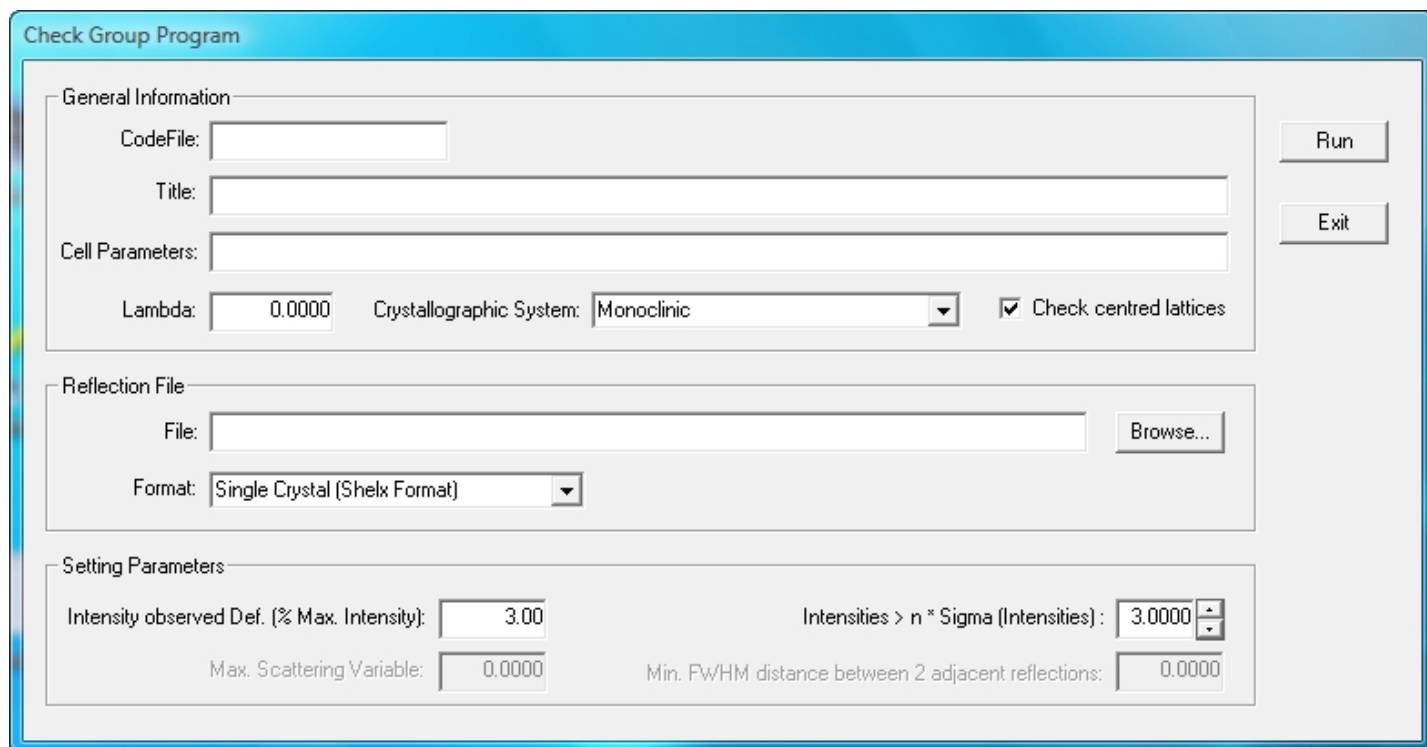
The group used for generating the reflections within *FullProf* should be the *holohedral group* of the crystal system in order to be sure that all possible reflections have been generated.

Running the program

You can run *CheckGroup* as follows:

- From a console or terminal: ***Local_Prompt>*** *checkgroup <cr>*

- By clicking on the [icon] icon on the Toolbar of FullProf Suite

Then a dialog will be showed similar to this picture.

General Information

CodeFile
Common code of files for the run

Title
A character string used as a title for the run

Cell parameters
Cell parameters

Lambda
Wavelength

Crystallographic system
Select one crystallographic system from the list

Centred lattice
Active this option for centred lattice calculations

Reflection File

File
Complete the reflection name. This may be selected using the Browse button.

Format
Select the format type of the reflection file

Setting Parameters

Intensity observed Def. (% Max. Intensity)
This is the threshold for considering as observed a particular reflection. Putting "1" means that all reflections having an intensity greater or equal to $0.01*Imax$ are considered as observed

Intensity > n * sigma (Intensity)
This is the threshold for considering as observed a particular reflection

Max. Scattering Variable
Enter a positive value indicating the maximum value of the Scattering angle

Min. FWHM distance between two adjacent reflections
Enter a real number. Then reflections are considered as distinguishable if their positions are separated at least dfw*FWHM
degrees in 2θ

Input File

The heading of a hkl-file has the form:

```
Pattern#  1 Phase No:   1  phase 1: Myphase
1366         0  293.00     <-- The number of effective reflections may be lower
   2   0   0    4       18.884           0.801        5.1224          0.0138
   1   1   2    8       27.160           0.473        5.4115          0.0138
   2   0   1    8      403.671           1.470        5.5030          0.0138
   2   1   0    8        4.917           0.551        5.7275          0.0139
  .............
```

The two first lines are considered by the program as comments. The rest of lines contain the following items:
- h,k,l
- Mult
- Intensity
- Sigma
- 2θ
- FWHM

Output File

After running the program, two files, one with extension **SPG** and the other with extension **CFL**, are generated.

The **SPG** file contains the results and the **CFL** summarizes the answer to the questions with keywords. This last file can be modified and used as input to the program that can be invoked in a third way as:

Local prompt> *check_group* *-f* *my_cfl_file*

where "my_cfl_file" is the name of the **CFL** file without extension.

Bibliography