Keywords on CFML

# Block definitions

|  |
| --- |
| **BLOCKNAME\_**StringIdentification **N**  **…**  **…**  **END\_BLOCKNAME\_**StringIdentification |

Examples:

|  |
| --- |
| **PHASE\_**PbSO4 **1**  **…**  **…**  **END\_PHASE\_**PbSO4 |

|  |
| --- |
| **PATTERN\_**Xray **1**  **…**  **…**  **END\_PATTERN\_**Xray |

Exceptions:

Exists an exception for a particular COMMANDS block.

|  |
| --- |
| **COMMANDS**  **…**  **…**  **END\_COMMANDS** |

# Pattern Block

***Background definitions***

In this case, the information for Backgrounds will be using a subblock definition according to general definition of the blocks.

|  |
| --- |
| **BACKGD**  Method [N1]  **…**  **…**  **END\_BACKGD** |

The available methods are:

* Linear\_interpolation
* Spline\_interpolation
* Polynomial
* Chebychev
* Peaks\_pVoigt
* Peaks\_Split\_pVoigt

Example:

Texto

Descripción generada automáticamente

Internally, the user can define zones of different procedures, where the first line will be the indication of the background model followed by the number of parameters to be read.

Example:

Texto, Carta

Descripción generada automáticamente

***Exclude regions***

We can define a exclude regions for different type of calculations. We’ll use also a particular subblock into the pattern block

|  |
| --- |
| **EXCLUDE\_REGIONS**  Start Finish ! Region 1  …  Start Finish ! Region …  **END\_EXCLUDE\_REGIONS** |

# Command Zone

Within a CFL file, a command zone can be created (for the momento this must be unique) to define certain instructions (or directives) to the program that have to interpret the actions indicated.

This command area is defined as follows:

|  |
| --- |
| **COMMANDS**  **… line …**  **…**  **…**  **… line …**  **END\_COMMANDS** |

Inside of this zone, we can define different subblocks (mainly for patterns or phases) following the general rules with the exception to give a numer that it is only used when we define them outside of command zone.

|  |
| --- |
| **COMMANDS**    **PATTERN\_***XrayPatt*  **…**  **…**  **END\_PATTERN\_***XrayPatt*    **PHASE\_***PhName*  **…**  **…**  **END\_PHASE\_***PhName*    **END\_COMMANDS** |

In this area, we can give a set of instructions to perform the required actions. In principle, it is intended to carry out actions to activate refinement parameters, add constraints/restraints conditions.

**Instructions**

The next directives are currently operatives:

**VARY**

**VARY CELL XYZ UISO …**

**VARY Z\_O3**

**VARY XYZ\_O1\_PHAS2**

**VARY ALL Ti1 O1**

**FIX**

Same behaviour that VARY

**EQUAL**

**EQUAL UISO O**

**EQUAL UISO O1 O2 Value O3 Value …**

**EQUAL X\_O1 X\_O1\_PHAS2 Value X\_O1\_PHAS3 Value …**

**DFIX**

Distance restraints

**DFIX** *Value [Sigma]* **AtNam1A AtNam1B […AtNamA AtNamB]**

**DFIX** 0.960 0.005 **C1 H1 C2 H2 C3 H3 C4 H4**

**AFIX**

Angle restraints

**AFIX** *Value [Sigma]* **AtNam1A AtNam1B AtNam1C […AtNamA AtNamB AtNamC]**

**AFIX** 90.0 0.1 **O1 Ca1 O2**

**TFIX**

Torsional angle restraints

**TFIX** *Value [Sigma]* **AtN1A AtN1B AtN1C AtN1D […AtNA AtNB AtNC AtND]**

**TFIX** 30.0 0.1 **C1 C2 C3 C4**

Note:

***Restraints***

Is possible use a symmetry information on atoms name including the code [ **\_N.IJK** ] where:

**N**: Number of symmetry operator to apply in the coordinates of the atom

**I J K**: Traslation component (555, 465, 765, …)

***ATTENTION***

* Atoms labels are case sensitive

# **PATTERN Block**

**List of Directives**

|  |  |  |
| --- | --- | --- |
| 01 | **U** |  |
| 02 | **V** |  |
| 03 | **W** |  |
| 04 | **UVW** |  |
| 05 | BKG1 |  |
| 06 | BKG2 |  |
| 07 | BKG3 |  |
| 08 | BKG4 |  |
| 09 | BKG5 |  |
| 10 | BKG6 |  |
| 11 | BKG7 |  |
| 12 | BKG8 |  |
| 13 | BKG9 |  |
| 14 | BKG10 |  |
| 15 | BKG11 |  |
| 16 | BKG12 |  |
| 17 | BKG |  |
| 18 | SC1 |  |
| 19 | SC2 |  |
| 20 | SC3 |  |
| 21 | SC |  |
| 22 | EXTI1 |  |
| 23 | EXTI2 |  |
| 24 | EXTI3 |  |
| 25 | EXTI |  |
| 26 | **ZERO** |  |
| 27 | **SYCOS** |  |
| 28 | **SYSIN** |  |
| 29 | LAMBDA |  |
| 30 | SD |  |
| 31 | SL |  |
| 32 | SDSL |  |
| 33 | DTT1 |  |
| 34 | DTT2 |  |
| 35 | SIG0 |  |
| 36 | SIG1 |  |
| 37 | SIG2 |  |
| 38 | SIG |  |
| 39 | GAM0 |  |
| 40 | GAM1 |  |
| 41 | GAM2 |  |
| 42 | GAM |  |

# **PHASE Block**

**List of Directives**

|  |  |  |
| --- | --- | --- |
| 01 | **A** |  |
| 02 | **B** |  |
| 03 | **C** |  |
| 04 | **ALPHA** |  |
| 05 | **BETA** |  |
| 06 | **GAMMA** |  |
| 07 | **CELL** |  |
| 08 | **X** |  |
| 09 | **Y** |  |
| 10 | **Z** |  |
| 11 | **XYZ** |  |
| 12 | **OCC** |  |
| 13 | **UISO** |  |
| 14 | **U** |  |
| 15 | **U11** |  |
| 16 | **U22** |  |
| 17 | **U33** |  |
| 18 | **U12** |  |
| 19 | **U13** |  |
| 20 | **U23** |  |
| 21 | RX |  |
| 22 | RY |  |
| 23 | RZ |  |
| 24 | IX |  |
| 25 | IY |  |
| 26 | IZ |  |
| 27 | RM |  |
| 28 | RPHI |  |
| 29 | RTHE |  |
| 30 | IM |  |

**List of Directives**

|  |  |  |
| --- | --- | --- |
| 31 | IPHI |  |
| 32 | ITHE |  |
| 33 | MAGPH |  |
| 34 | XC |  |
| 35 | YC |  |
| 36 | ZC |  |
| 37 | CENTRE |  |
| 38 | THE |  |
| 39 | PHI |  |
| 40 | CHI |  |
| 41 | ORIENT |  |
| 42 | T |  |
| 43 | L |  |
| 44 | S |  |
| 45 | TL |  |
| 46 | LS |  |
| 47 | TS |  |
| 48 | TLS |  |
| 49 | SIZE |  |
| 50 | STRAIN |  |
| 51 | SCALE |  |
| 52 | **ALL** | Only for XYZ and UISO using Atom’s label |
| 53 |  |  |
| 54 |  |  |
| 55 |  |  |
| 56 |  |  |
| 57 |  |  |
| 58 |  |  |
| 59 |  |  |
| 60 |  |  |

NOT YET IMPLEMENTED

List of Directives

|  |
| --- |
| **FILE** Type\_of\_file Format Name \_of File |

Type of file:

**Powder** Powder diffraction file

**Intensities** Integrated intensidites file

**Irf** Instrumental resolution file

Format:

Xye, xys, socabim, old\_d1a, g41, panlaytical, …

If the type of file is IRF then you have to give a number indicating the type of IRF

Example:

FILE POWDER XYS *Neutron\_Pattern.xys*

FILE INTENSITIES *HoBaCuO.int*

|  |
| --- |
| **LAMBDA** Symbol [Monocromatic]  *or*  value1 [value2] |

Wavelength of the radiation

|  |
| --- |
| **PATT\_TYPE** radiation\_type options |

Define the type of radiation of the pattern

Radiation type:

**Neutrons** For neutrons radiations

X-**Rays** X-ray diffraction

In the case of neutrons, then

Options:

**CW** or **TOF**

|  |
| --- |
| **PROFILE** FunctionName |

Define the profile function to be used

Names:

TCH\_pVoigt

Lorentizian

Gaussian

|  |
| --- |
| **RANGE** min max step |

Define the range of the pattern dataset

|  |
| --- |
| **SYCOS** value |

In case of constant wave (CW) correct the sample displacement in θ-2θ diffractometers

|  |
| --- |
| **SYSIN** value |

In case of constant wave (CW) correct the sample transparency in θ-2θ diffractometers

|  |
| --- |
| **UVWX** value1 value 2 value3 value4 |

Caglioti function definition

|  |
| --- |
| **ZERO** value |

Define the zero point of the pattern