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** |

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

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

Caglioti function definition

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

Define the zero point of the pattern

**PHASE\_**PhaseName N

**END\_PHASE\_**PhaseName

|  |  |
| --- | --- |
| A  B  C  ALP  BET  GAM  CELL | %Phase 1  Vary a b c  %EndPhase  %Phase 2  Vary cell  %EndPhase  %Phase  Vary cell\_phas1  %EndPhase |
|  |  |

# Command Zone

Dentro de un fichero CFL puede crearse una zona de comandos (de momento ésta debe ser única) para definir ciertas instrucciones al programa que deba interpretar las acciones indicadas en esta zona de comandos o directivas.

Esta zona de comandos se define de la siguiente manera:

**COMMANDS**

**… line …**

**… line …**

**END\_COMMANDS**

De esta forma, se delimitará las líneas en las que se debe buscar las acciones a realizar. La rutina en cuestión se llama ***Get\_ZoneCommands*** . El procedimiento devuelve el número de comienzo y final de esta zona sin tener en cuenta COMMANDS / END\_COMMANDS

***Observación:*** *Podemos definir un fichero CFL como una zona de comandos en su totalidad por lo que no haría falta llamar a* ***Get\_ZoneCommands*** *puesto que la línea inicial y final son la inicial y final del propio fichero*.

***Blocks dentro de la Zona de Commandos***

Dentro de la zona de comandos podemos hacer referencia a diferentes bloques (Patterns, Phases, etc) y para ello deberemos utilizar las siguientes directivas:

**%BlockType** *BlockName*

**… line …**

**… line …**

**%End\_BlockType**

Se debe verificar que:

* El identificador *BlockName* es un literal que se usa para identificar dicho bloque y no debe contener espacios. Debe ser único.
* El uso de bloques es obligatorio en el caso que deseemos trabajar con diferentes fases, patrones de difracción, moléculas, etc….
* Existe un orden de prevalencia definida:

Phase > Pattern > Molec > Atoms

* Un bloque puede contener la definición de otros bloques, pero no pueden ser del mismo tipo. Es decir, un bloque pattern no puede contener otro bloque del tipo pattern. En general, las limitaciones entre bloques sería la siguiente:
  + Bloque (phase): Puede contener bloques del tipo pattern, molec y atoms
  + Bloque (pattern): No pude contener ningún bloque
  + Bloque (molec): Puede contener bloque del tipo atoms
  + Bloque (atoms): No puede contener ningún tipo de bloque

# Pattern Block

|  |
| --- |
| %Pat[tern] [N]  ….  %EndPat[tern] |

Note: If N is given, then all references are associated to the respective Pattern|Phase,….

|  |  |
| --- | --- |
| U  V  W  UVW | %Pattern  Vary UVW\_Pat1  Fix U\_Pat1  %EndPattern |
|  |  |
| BKG  BKG[1…12] | % Pattern 2  Vary BKG1 BKG2 BKG3  %EndPattern |
|  |  |
| SC  SC[1…3] | … |
|  |  |
| EXTI  EXTI[1…3] | … |
|  |  |

# Phase Block

|  |
| --- |
| %Pha[se] [N]  ….  %EndPha[se] |

|  |  |
| --- | --- |
| A  B  C  ALP  BET  GAM  CELL | %Phase 1  Vary a b c  %EndPhase  %Phase 2  Vary cell  %EndPhase  %Phase  Vary cell\_phas1  %EndPhase |
|  |  |

# Molecule Block

|  |
| --- |
| %Mol[ec] [N]  ….  %EndMol[ec] |

MOLECULE

|  |  |
| --- | --- |
| XC  YC  ZC  CENTRE | %molec  Vary centre  %endmolec |
|  |  |
| THE  PHI  CHI  ORIENT | %molec  Vary orient  %endmolec |
|  |  |
| T  L  S  TL  LS  TS  TLS | %molec  Vary TLS  %endmolec |
|  |  |

# Rigid Block

|  |
| --- |
| %RGB [N]  ….  %EndRGB[e] |

ATOMS

|  |  |  |  |
| --- | --- | --- | --- |
| ***Key*** | ***Reference*** | ***Format*** | ***Examples*** |
| FIX  VARY | X | Ref1[…RefN] Chem1[… ChemN]  Ref1[…RefN] Atm1[…AtmN]  Ref1\_Atm1[…RefN\_AtmN]  Ref\_PH1  Atm1\_PH1 | VARY ALL C H O  VARY XYZ U Pr1 Pr2  FIX OCC\_O2 X\_La1  VARY XYZ\_O1A\_PH2  FIX OCC\_PH1 O |
| Y |
| Z |
| XYZ |
| EQUAL |  | Ref1[…RefN] Chem1[…ChemN]  {Ref1\_Atm1 Ref2\_Atm2 [Mult] } | EQUAL UISO O  EQUAL XYZ O1 O2 (\*)  **(\*) Occ should be modified**  EQUAL X\_O1 X\_O2 0.5 |
|  | OCC |
|  |  |
|  | U |  |  |
|  | UISO |  |  |
|  | U11 |  |  |
|  | U22 |  |  |
|  | U33 |  |  |
|  | U12 |  |  |
|  | U13 |  |  |
|  | U23 |  |  |
|  |  |  |  |
|  | ALL |  |  |
|  |  |  |  |
|  | \_PH[n] |  |  |
|  | \_MOL[n] |  |  |

***Restraints***

DFIX value [sigma] AtNam1A AtNam1B […] [AtNamNA AtNamNB]

AFIX value [sigma] AtNam1A AtNam1B AtNam1C […] [AtNamNA AtNamNB AtNamNC]

TFIX value [sigma] At1A At1B At1C At1D […] [AtNA AtNB AtNC AtND]

MAGNETIC ATOMS

|  |  |
| --- | --- |
| RX\_ |  |
| RY\_ |  |
| RZ\_ |  |
| IX\_ |  |
| IY\_ |  |
| IZ\_ |  |
|  |  |
| RM\_ |  |
| RPHI\_ |  |
| RTHE\_ |  |
| IM\_ |  |
| IPHI\_ |  |
| ITHE\_ |  |
|  |  |
| MAGPH\_ |  |
|  |  |
| C1\_...C12\_ |  |
|  |  |

MOLECULE

|  |  |
| --- | --- |
| XC\_ |  |
| YC\_ |  |
| ZC\_ |  |
| CENTE\_ |  |
|  |  |
| THE\_ |  |
| PHI\_ |  |
| CHI\_ |  |
| ORIEN\_ |  |
|  |  |
| \_MOL[N] |  |
|  |  |

RIGID BODY BLOCK

|  |  |
| --- | --- |
| T\_ |  |
| L\_ |  |
| S\_ |  |
| TL\_ |  |
| TLS\_ |  |
|  |  |
| \_RGB[N] |  |
|  |  |

PHASES

|  |  |
| --- | --- |
| A |  |
| B |  |
| C |  |
| ALP |  |
| BET |  |
| GAM |  |
| CELL |  |
|  |  |
| PH[N] |  |
|  |  |

YSIZE

GSIZE

XSTRAIN

USTRAIN

PATTERNS

|  |  |
| --- | --- |
| U |  |
| V |  |
| W |  |
| UVW |  |
|  |  |
| BKG |  |
| BKG[N] | 1…6 |
|  |  |
| SC |  |
| SC[N] | 1..3 |
| EXTI |  |
| EXTI[N] | 1…6 |
|  |  |
|  |  |
|  |  |
|  |  |

PROPAGATION VECTORS

|  |  |
| --- | --- |
| KV\_ |  |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |

MICROABSORPTION (Pattern)

|  |  |
| --- | --- |
| MABS\_ |  |
| P0\_ |  |
| CP\_ |  |
| TAU\_ |  |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |

CONSTANT WAVELENGTH (Pattern)

|  |  |
| --- | --- |
| ZERO |  |
| SYCOS |  |
| SYSIN |  |
| RATIO |  |
|  |  |
|  |  |

TOF

|  |  |
| --- | --- |
| ZERO |  |
| DTT1 |  |
| DTT2 |  |
| ZT |  |
| DTT1T |  |
| DTT2T |  |
| XCROSS |  |
| WIDTH |  |
|  |  |
|  |  |

RESTRAINTS

DFIX[\_MOLN][\_PHAN] Value [V\_Std] {Object1 Object2}

AFIX[\_MOLN][\_PHAN] Value [V\_Std] {Object1 Object2 Object3}

TFIX[\_MOLN][\_PHAN] Value [V\_Std] {Object1 Object2 Object3 Object4}

Object: AtomLabel[\_N.IJK]

N: Number of symmetry operator IJK: Traslation component (555,465,…)