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:

**COMMANDS**

….

…

**END\_COMMANDS**

# Phase Block

**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,…)