Keywords on CFML

# Defining Blocks

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

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

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

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

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

# General instructions

* No se puede usar referencias globales e individuales al mismo tiempo

VARY XYZ O1 O2 UISO\_Fe

* No se puede mezclar directivas que afecten a tomos con Patterns o Fases

VARY CELL XYZ O P

# Defining Blocks

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

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] |  |
|  |  |
| SC |  |
| SC[N] |  |
| EXTI |  |
| EXTI[N] |  |
|  |  |
|  |  |
|  |  |
|  |  |

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,…)