Keywords on CFML

ATOMS

|  |  |  |  |
| --- | --- | --- | --- |
| ***Key*** | ***General…*** | ***Individual*** | ***Examples*** |
| FIX | X | Chemical symbol | VARY ALL C H O |
|  | Y | Atom\_Name | VARY U Pr1 |
| VARY | Z | Ref\_AtomName | FIX OCC\_O2 X\_La1 |
|  | XYZ | Ref\_AtomName\_Ref | VARY XYZ\_O1A\_PH2  FIX OCC O\_PH1 |
|  |  |  |  |
|  | OCC |  |  |
|  |  |  |  |
|  | U |  |  |
|  | UISO |  |  |
|  | U11 |  |  |
|  | U22 |  |  |
|  | U33 |  |  |
|  | U12 |  |  |
|  | U13 |  |  |
|  | U23 |  |  |
|  |  |  |  |
|  | ALL |  |  |
|  |  |  |  |
|  | PH[n] |  |  |
|  | MOL[n] |  |  |

***Description:***

VARY XYZ [OCC][U\_ISO] AtName1 AtName2

VARY U\_ISO MOL1

VARY X\_AtName1 OCC\_AtName2

FIX XYZ H -> Fix all coordinates for H atoms

VARY XYZ O C -> Refinable all coordinates for O and C atoms

Not allowed to use global and local directives at the same time

***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]\_ |  |
|  |  |
| \_PAT[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,…)